Simulating monolithic active pixel sensors

A technology-independent approach using generic doping profiles

H. Wennlöf

for the Tangerine collaboration

20/6 -24

The Tangerine collaboration at DESY: A. Chauhan, M. Del Rio Viera, J. Dilg, D. Eckstein, F. Feindt, I.-M. Gregor, Y. He, K. Hansen, L. Huth, S. Lachnit, L. Mendes, B. Mulyanto, D. Rastorguev, C. Reckleben, S. Ruiz Daza, J. Schlaadt, P. Schütze, A. Simancas, S. Spannagel, M. Stanitzki, A. Velyka, G. Vignola, H. Wennlöf

Outline

- Motivation
    - Why simulations?
- Simulation tools
    - TCAD
    - Allpix Squared
- Simulation procedure
    - Examples from the Tangerine project
        - Procedure applicable in many cases, however
- Example results
- Conclusions and outlook
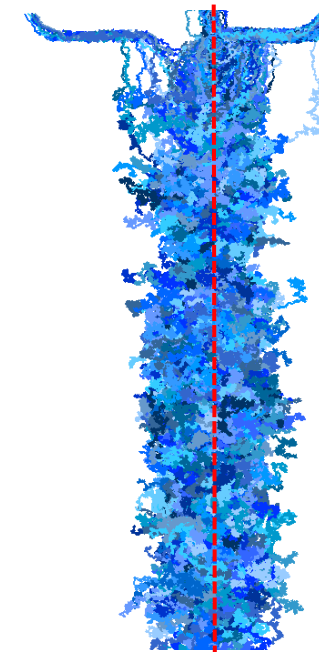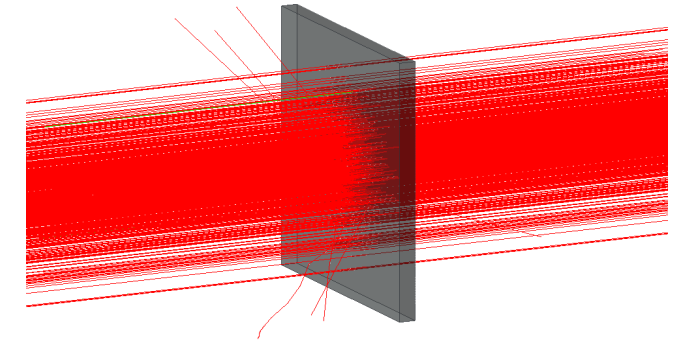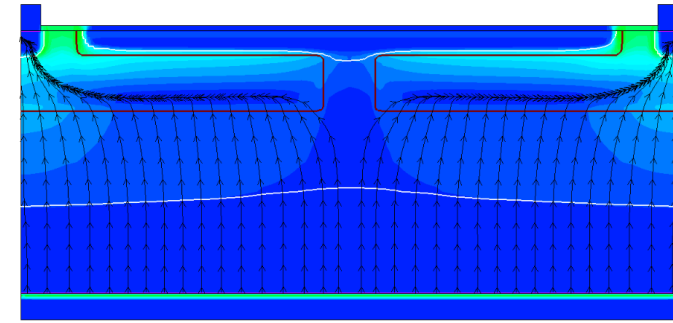
Silicon sensor simulations

- **Goal:** Accurate simulation of the **charge collection behaviour** in the sensitive volume

  - Enables **understanding and prediction of sensor performance** (e.g. resolution, efficiency)

  - Done by simulating the **movement of electron-hole pairs** created by an interacting particle

- **Issue:** The access to manufacturing process information may be **very limited**

  - The Tangerine project for example utilises a commercial CMOS imaging process - detailed process information is **proprietary**

- **Solution:** development of a **technology-independent simulation approach using generic doping profiles**

  - Currently writing a **paper** describing the approach, serving as a **toolbox** for such simulations
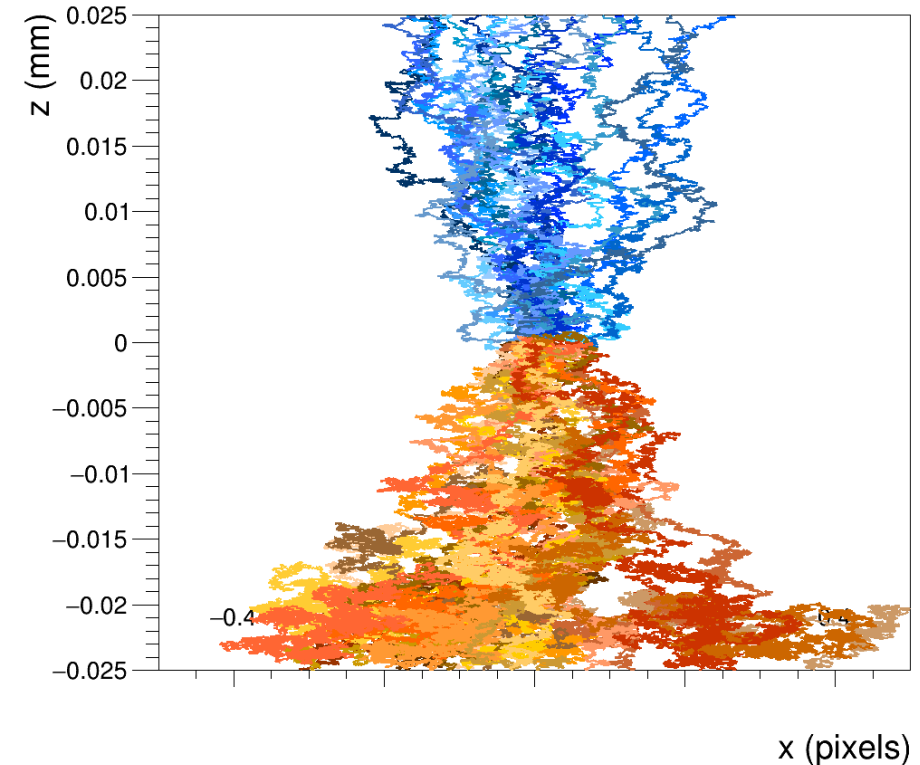
Simulated motion of individual electrons and holes deposited in the centre of a silicon sensor with a linear electric field

Simulating Monolithic Active Pixel Sensors:
A Technology-Independent Approach Using Generic Doping Profiles

Håkan Wennlöf[a,*], Dominik Dannheim[b], Manuel Del Rio Viera[a,1], Katharina Dort[b,1], Doris Eckstein[a], Finn Feindt[a], Ingrid-Maria Gregor[a], Lennart Huth[a], Stephan Lachnit[a,1], Larissa Mendes[a,1], Daniil Rastorguev[a,1], Sara Ruiz Daza[a,1], Paul Schütze[a], Adriana Simancas[a,1], Walter Snoeys[b], Simon Spannagel[a], Marcel Stanitzki[a], Alessandra Tomal[c], Anastasiia Velyka[a], Gianpiero Vignola[a,1]

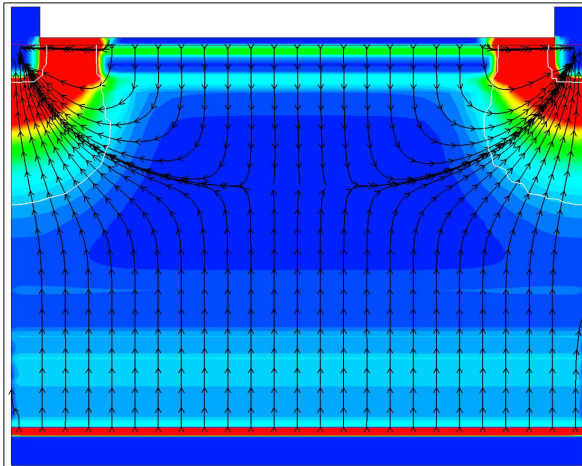[a]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany
[b]CERN, Geneva, Switzerland
[c]University of Campinas, Cidade Universitaria Zeferino Vaz, 13083-970, Campinas, Brazil
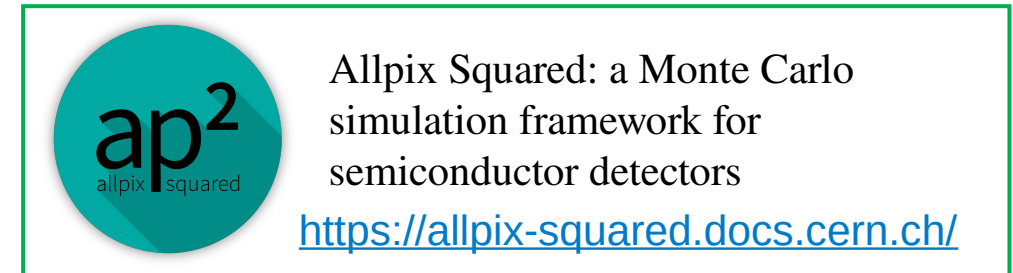
Tools used in the simulation approach

Sentaurus TCAD — **SYNOPSYS®** *Silicon to Software™*

Technology Computer-Aided Design

ap² allpix squared

Allpix Squared: a Monte Carlo simulation framework for semiconductor detectors

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

- Models semiconductor devices using **finite element methods**

- Calculates realistic and accurate **electric fields and potentials** from doping concentrations

- Simulates **full detector chain**, from energy deposition through charge carrier propagation to signal digitisation

  – Interfaces to **Geant4** and **TCAD**

- Simulation performed **quickly** - allows for **high-statistics** data samples across a full detector
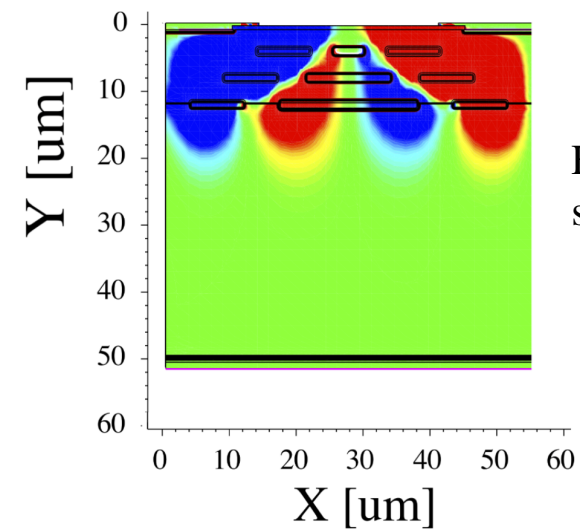
Example electric field in TCAD
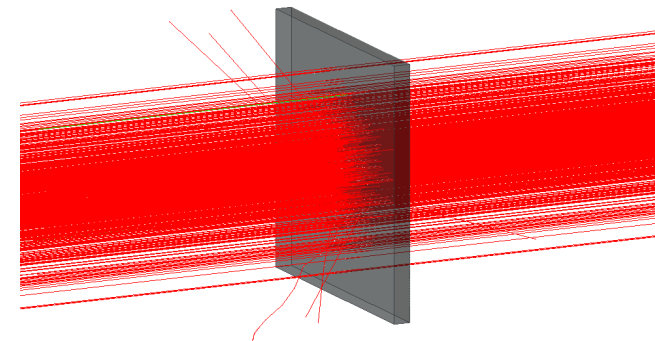
Particle beam passing through a single sensor in Allpix²

TCAD

Technology computer-aided design

Enhanced Lateral Drift sensor simulation, A. Velyka
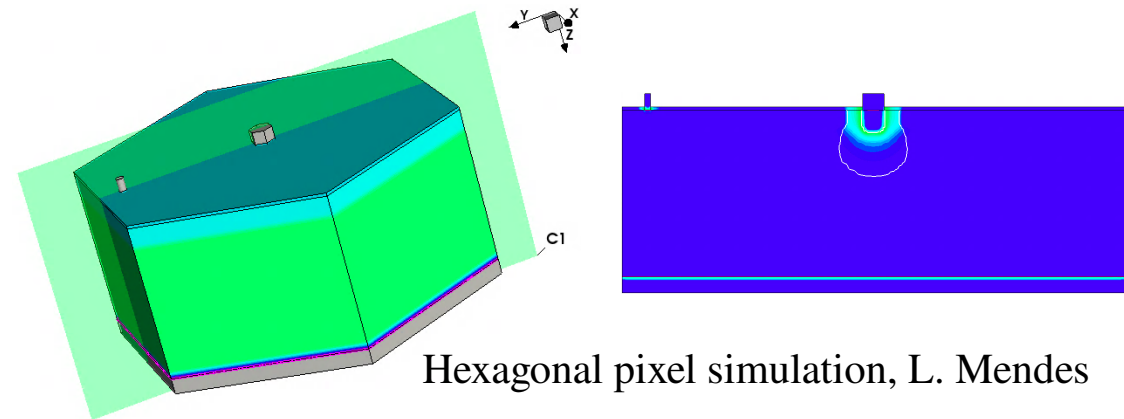
- Models **semiconductor devices** in 2D or 3D, and numerically solves equations using provided information

  - By providing doping information, e.g. **electric fields** and **weighting potentials** can be simulated

  - Capacitances, I-V and C-V curves, and transient properties can be extracted

- **Fabrication steps** in semiconductor manufacturing can be simulated

- Different pixel geometries and layouts can be simulated in **great detail**

- Some example resulting electric fields shown on the right

Hexagonal pixel simulation, L. Mendes
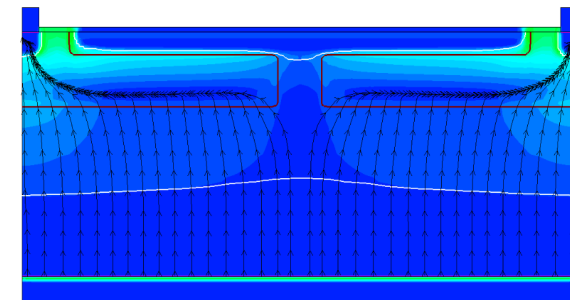
Rectangular pixel simulation, A. Simancas

Allpix Squared

A Monte Carlo simulation framework for semiconductor detectors

- Simulates **charge carrier motion** in semiconductors, using **well-tested** and **validated** algorithms
  - Includes different models for e.g. charge carrier mobility, lifetime and recombination, trapping and detrapping
  - Support for several semiconductor materials and pixel and sensor geometries
- Provides a **low entry barrier** for new users
  - Simulations are set up via **human-readable configuration files**
- **Steady development** over many years
  - Framework is **easily extendable** and **widely used**
  - **Open-source**, and written in **modern C++**
  - Version 3.1.0 released on May 17th of this year
- [User workshop](#) presentations hold many example applications

Website and documentation:
https://allpix-squared.docs.cern.ch/

```
[AllPix]
number_of_events = 10000
detectors_file = "telescope.conf"

[GeometryBuilderGeant4]
world_material = "air"

[DepositionGeant4]
particle_type = "Pi+"
number_of_particles = 1
source_position = 0um 0um -200mm
source_type = "beam"
beam_size = 1mm
beam_direction = 0 0 1

[ProjectionPropagation]

[SimpleTransfer]

[DefaultDigitizer]
```

Minimal simulation configuration example

Silicon simulation layout and assumptions

Using the Tangerine project as an example

- High-resistivity **epitaxial layer** grown on low-resistivity **substrate**

- Approximate doping concentrations can be found in **published papers** and theses, that have been approved by the foundry

  - The **exact values are proprietary information**, however (but we do not need them to model the sensor behaviour)

- Doping wells are simulated **without internal structure** and as flat profiles

  - Small collection n-well in the centre of the pixel

  - Deep p-well holding the in-pixel CMOS electronics

- **3D geometry** simulated, including **metal bias contacts** and **Ohmic contact regions** in the silicon
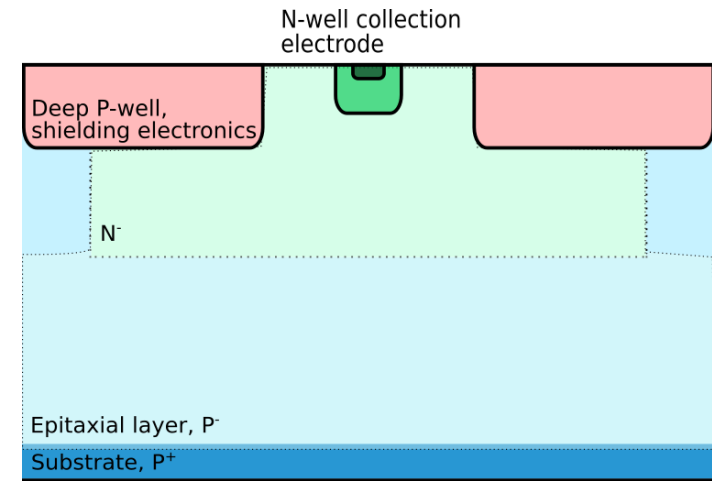

"N-gap layout", M. Münker et al 2019 JINST 14 C0501

Metal bias contacts
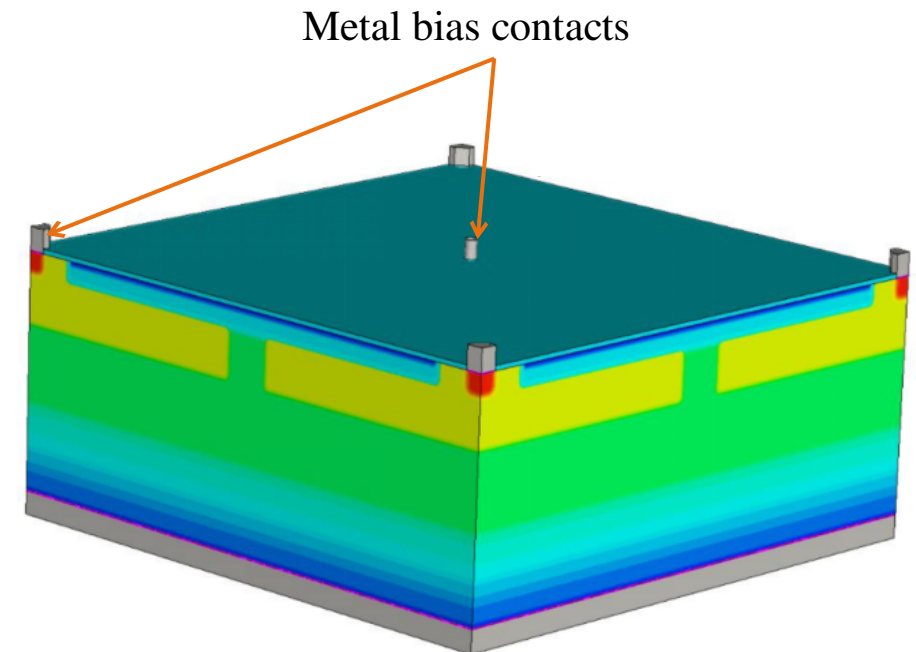
Finite element method simulations using TCAD

Using the [Tangerine project](#) as an example

- Using TCAD, **doping profiles** and **electric fields** are simulated
  - Studies are made observing the **impact of varying different parameters**, e.g. mask geometries

- Starting by creating the **geometry and doping regions**
  - Doping distribution is **further refined** by simulating diffusion between regions at reasonable **sensor production process temperatures**
    - Gives a continuous interface between epi and substrate

- Device simulations used to simulate **electric fields**, **electrostatic potentials**, **capacitances**, and performing **transient simulations**
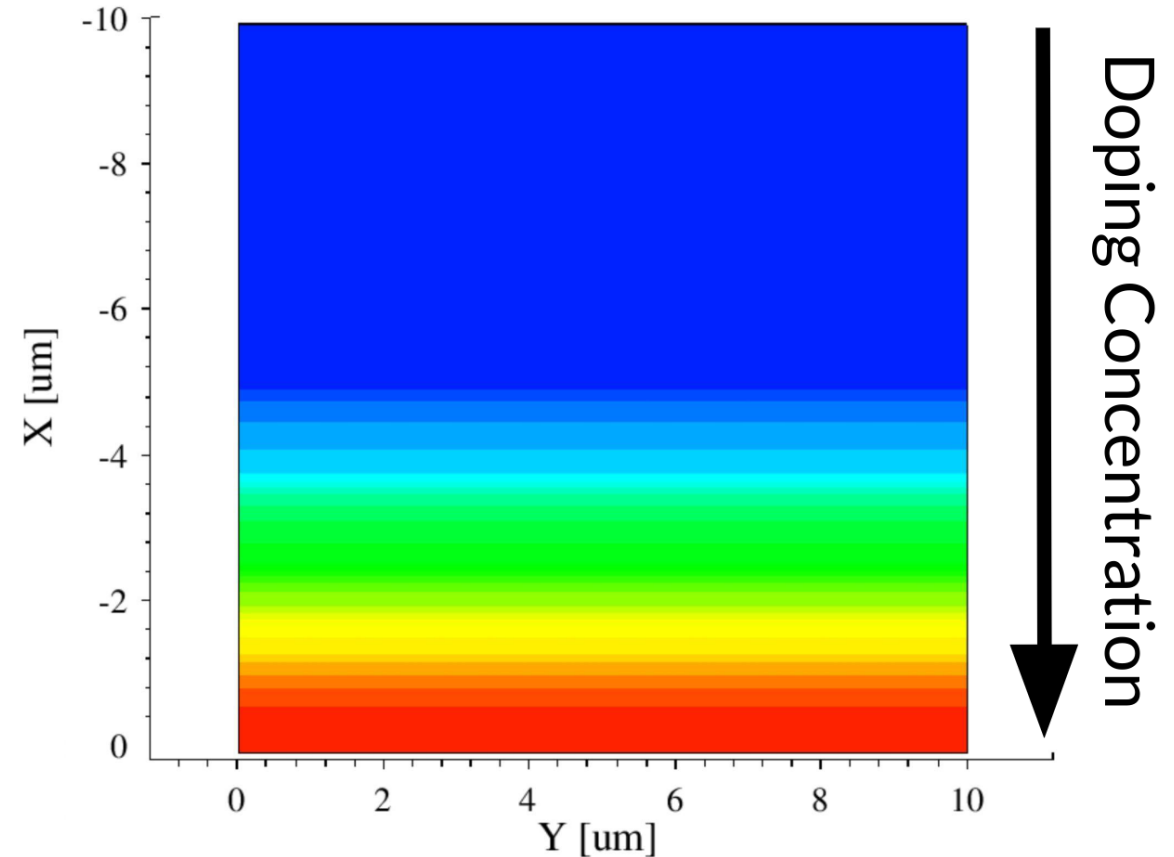

Process simulation result, showing dopant diffusion between substrate and epitaxial layer

Finite element method simulations using TCAD

**Example study: impact of n-gap size on electric field**

- The gap in the n-gap layout is introduced to give a **lateral electric field at pixel edges**

- The magnitude of the field depends on the **size of the gap**

    - Too small gap: the lateral field components **cancel out**

    - Too large gap: **low-field region** between pixels (i.e. in the gap)

- Figures show simulation results for the **lateral electric field** (red and blue) for different gap sizes

Collection electrodes   Gap   Depletion boundary

(a) 1 μm gap   (b) 2.5 μm gap   (c) 4 μm gap
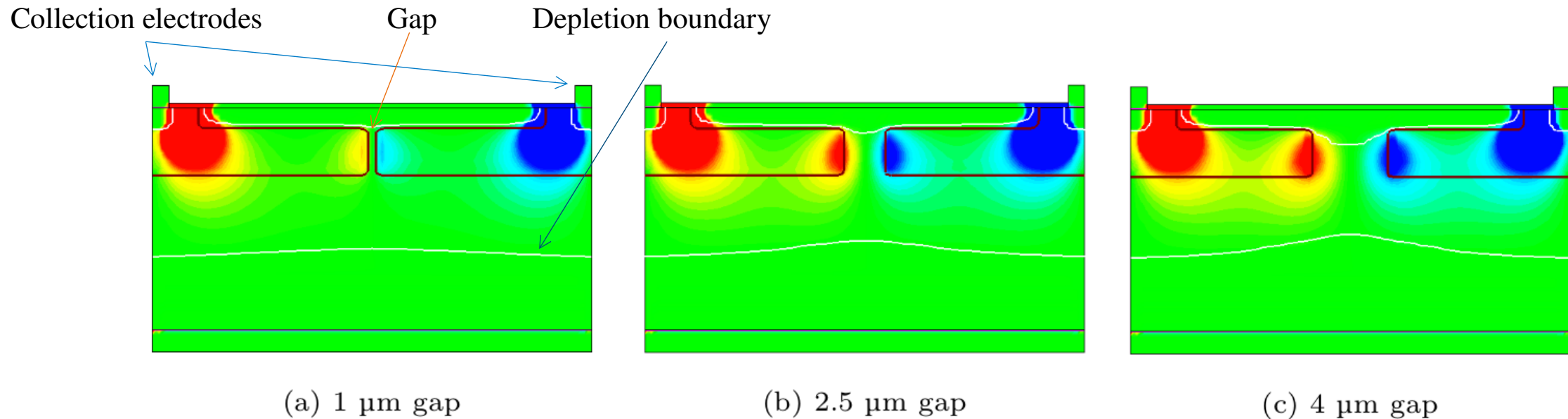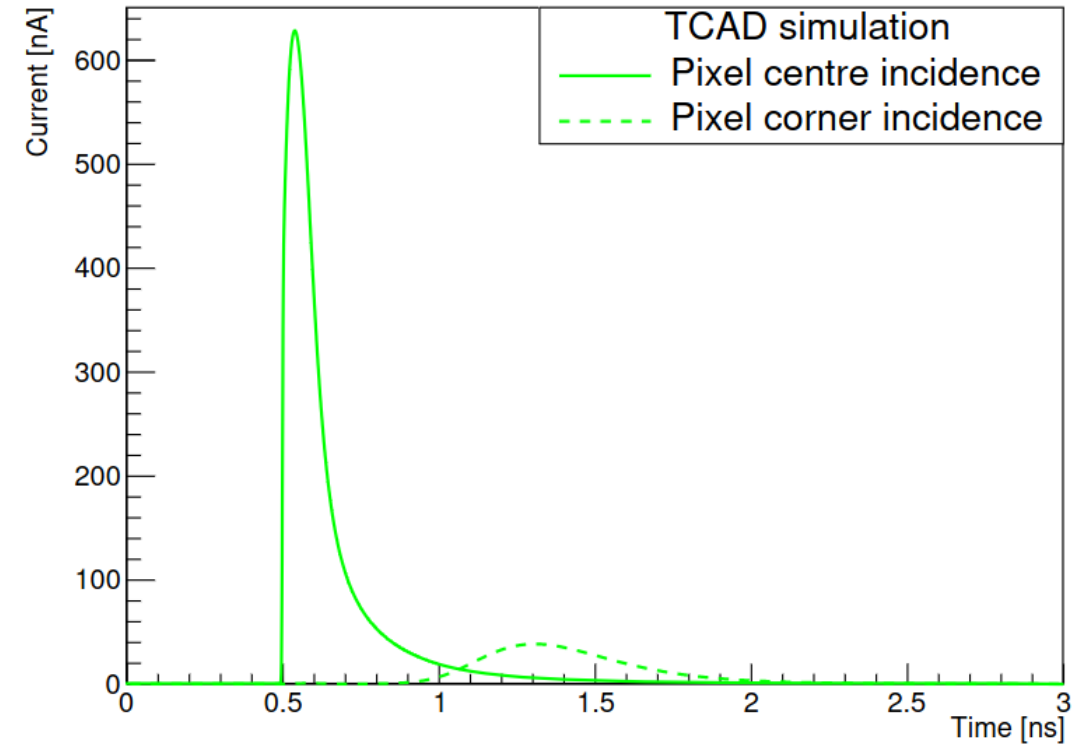
Finite element method simulations using TCAD

Transient simulations

- Extracting the **time-dependent induced signal** on the collection electrodes, from traversal of a MIP

- Investigating both **pixel corner** incidence and **pixel centre** incidence

 - Gives indication of "worst case" and "best case" particle hit scenarios
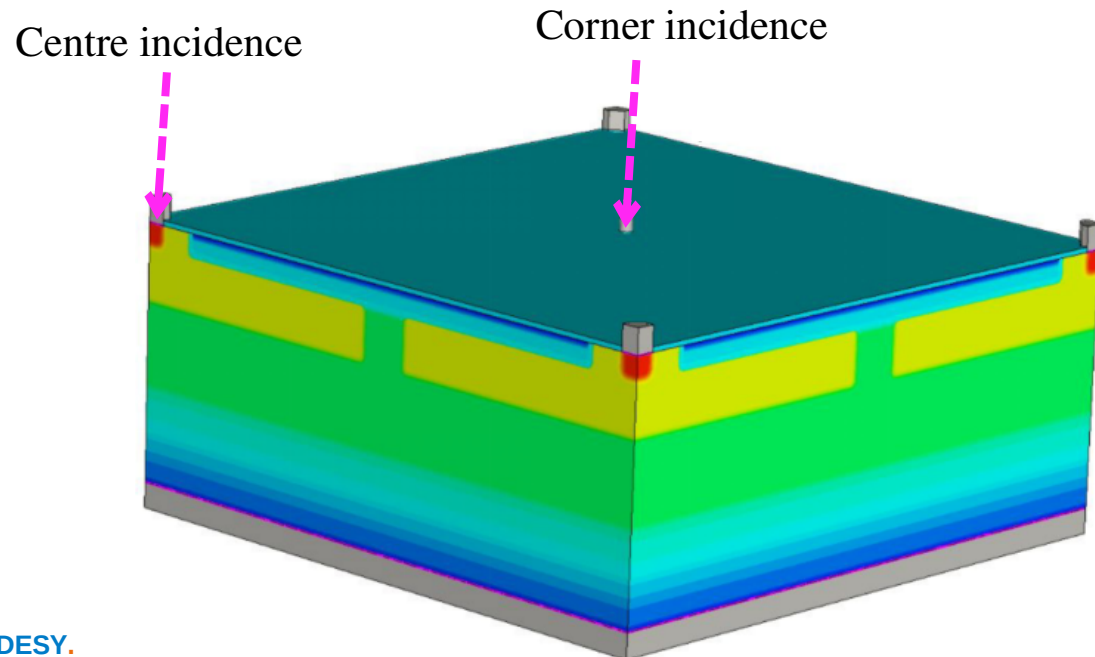
Centre incidence   Corner incidence

Transient pulses for pixel centre and corner incidence

Monte Carlo simulations using Allpix²

- **Flexible** and **modular** framework, describing each part of **semiconductor signal generation and propagation**

- Allows import of **TCAD fields and doping profiles**

  - Allpix² and TCAD make a **powerful combination**; fast and detailed simulations possible, allowing high statistics

Figure from S. Spannagel, BTTB10, and A. Simancas, 4th Allpix Squared User Workshop
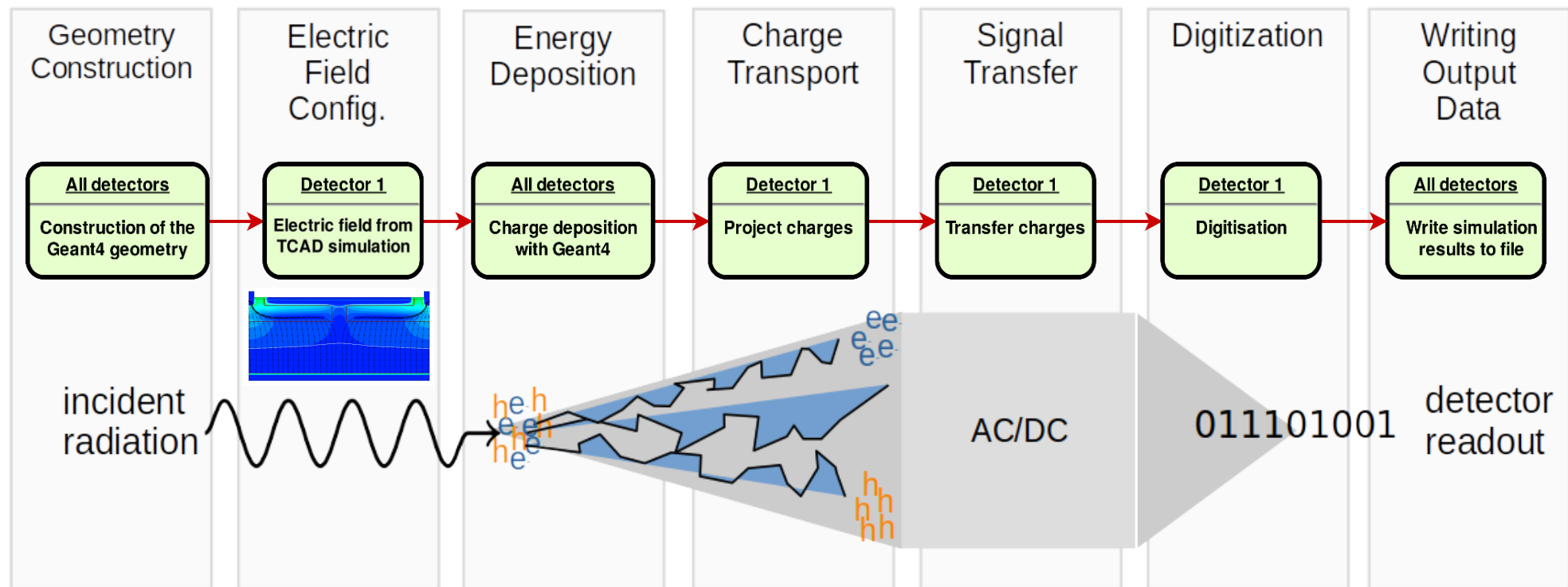
Monte Carlo simulations using Allpix²

Impact of mobility model

- Physical parameters and models can easily be **exchanged**

- Example: **mobility models** in silicon

  - Jacoboni-Canali model is **doping-independent**

    - Sufficient for describing charge propagation in low-doped regions

    - In high-doped regions (e.g. substrate) diffusion is unphysically large

  - Extended Canali model (including the Masetti model) is **doping-dependent**

    - Describes charge carrier motion well also in highly-doped regions

- Linegraphs show the **propagation paths of individual charge carriers**

 - Each blue line is the path of a single electron
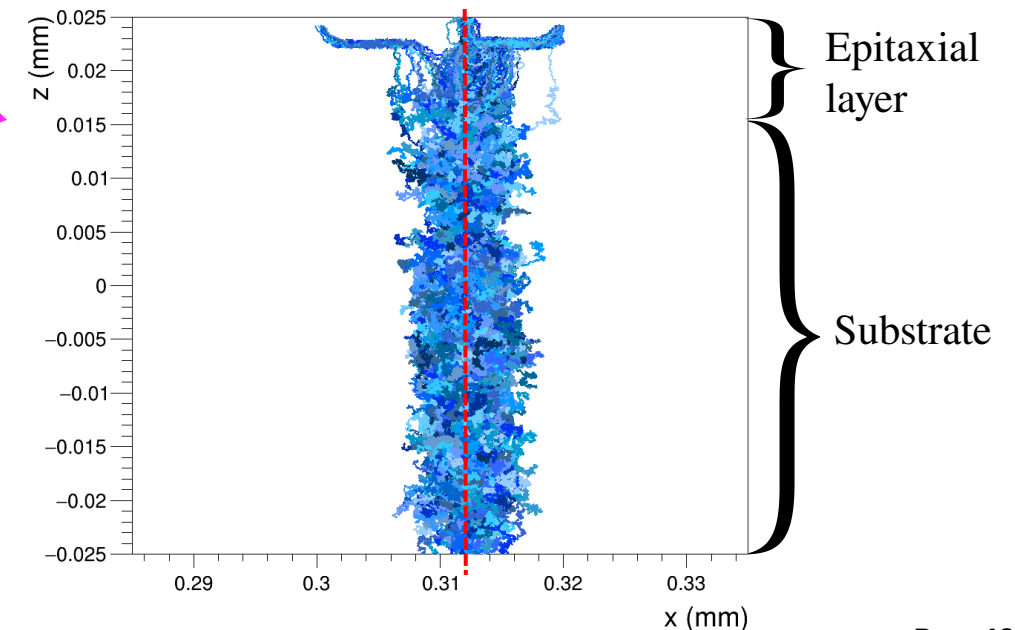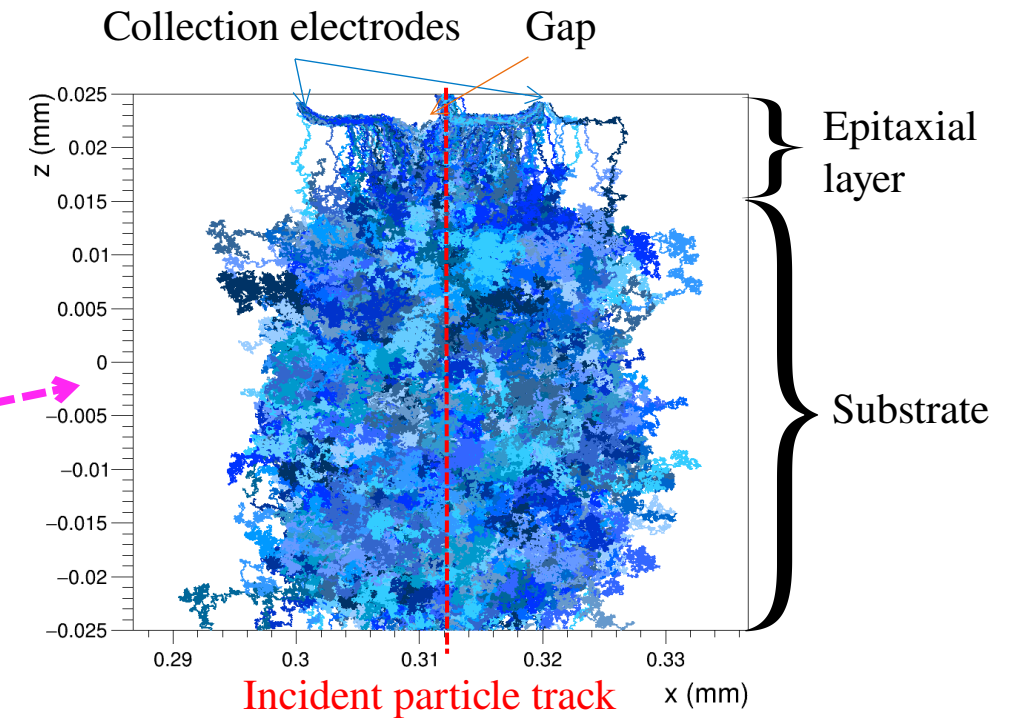
Allpix² combined with TCAD

Example result from the Tangerine project

- High-statistics simulations allow extraction of observables such as cluster size, resolution, efficiency

- Sensor **mean efficiency versus detection threshold**, for different bias voltage

  - Simulation carried out with a DESY II-like beam of electrons; many events (500 000), so statistical error bars are small

- The trend is as expected:

  - Efficiency **decreases as threshold increases**

  - The sensor reaches its **full efficiency** potential already at -1.2 V

- 0 V deviates from the others by being less efficient as threshold increases, most likely due to **incomplete depletion**
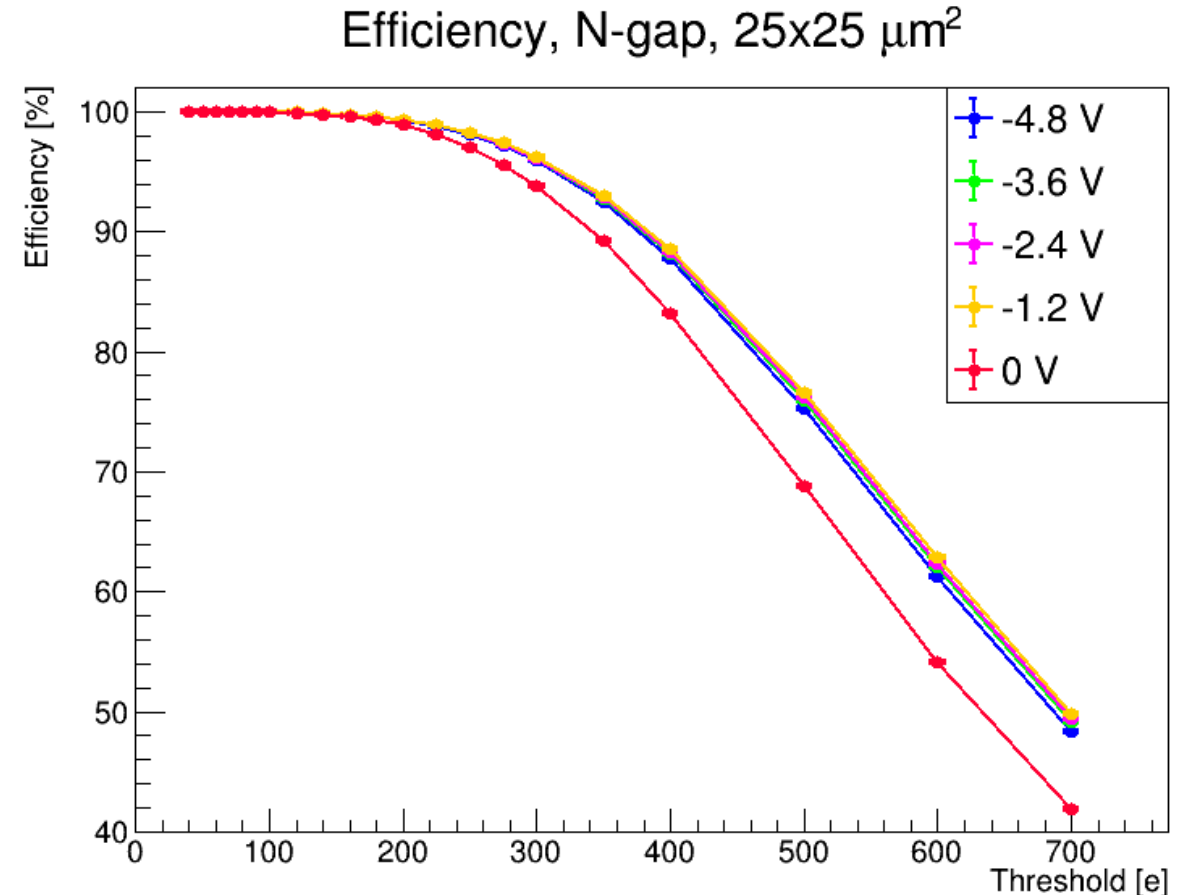
Simulations compared to data

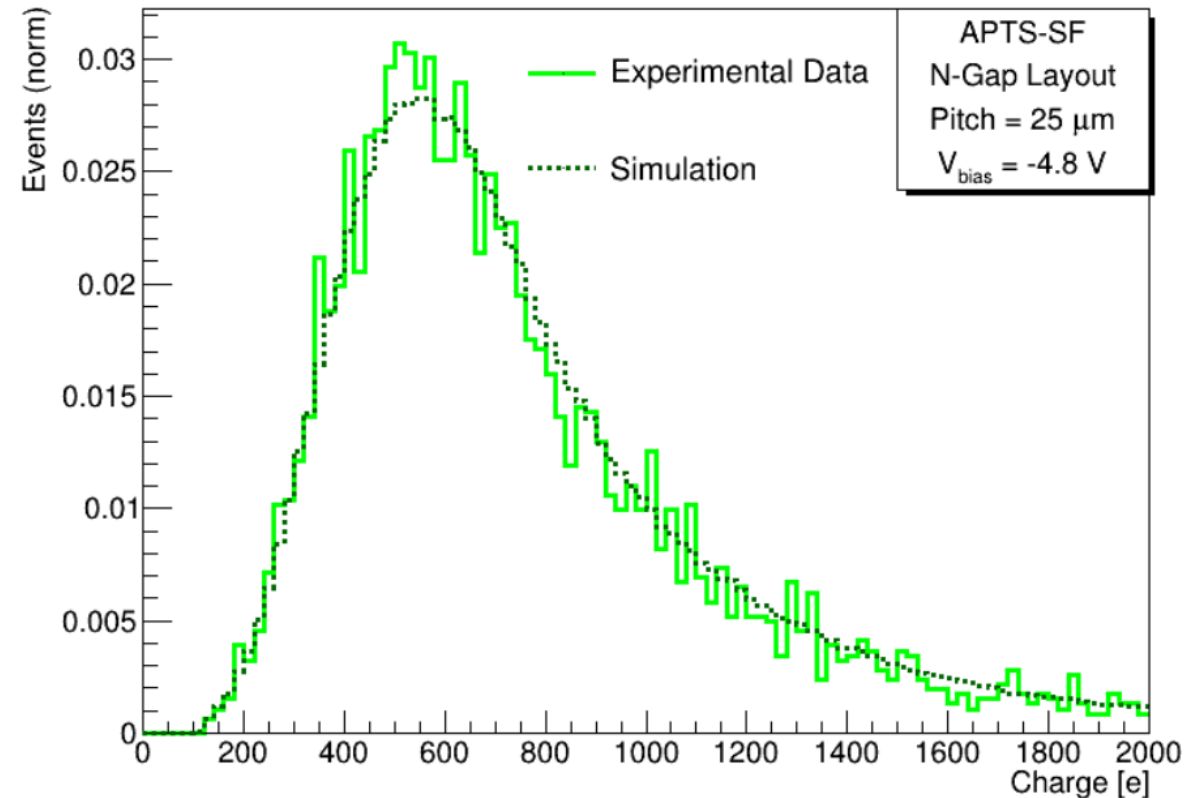**Does the procedure *actually* work?**
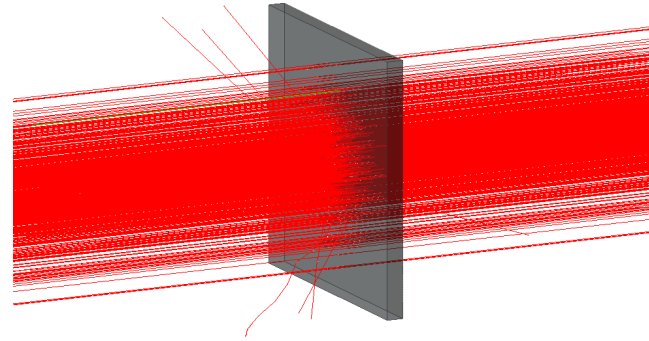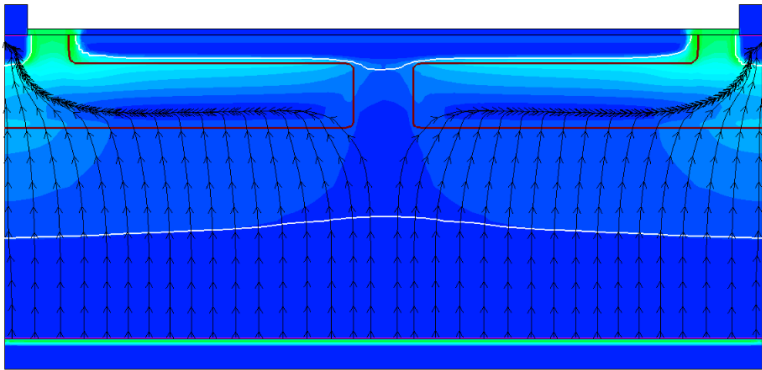
Allpix² combined with TCAD - Preliminary comparison to data

Example result from the [Tangerine project](#)

- Testbeams have been carried out at DESY, and comparisons made to simulations

- Results from the "Analog Pixel Test Structure" ([APTS](#))
  - N-gap layout
  - 25x25 μm^2 pixel size
  - 4x4 pixel matrix
  - -4.8 V bias voltage

- The trend between simulations and data **matches well**

Cluster charge distribution

https://doi.org/10.1016/j.nima.2024.169414

Allpix² combined with TCAD - Preliminary comparison to data

Example result from the [Tangerine project](#)

- Testbeams have been carried out at DESY, and comparisons made to simulations

- Results from the "Analog Pixel Test Structure" ([APTS](#))
  - N-gap layout
  - 25x25 μm² pixel size
  - 4x4 pixel matrix
  - -4.8 V bias voltage

- The trend between simulations and data **matches well**
  - Error bars on the simulated results are purely statistical here

- In conclusion, the developed **simulation procedure works well**, without any proprietary information

Mean efficiency vs threshold

https://doi.org/10.1016/j.nima.2024.169414
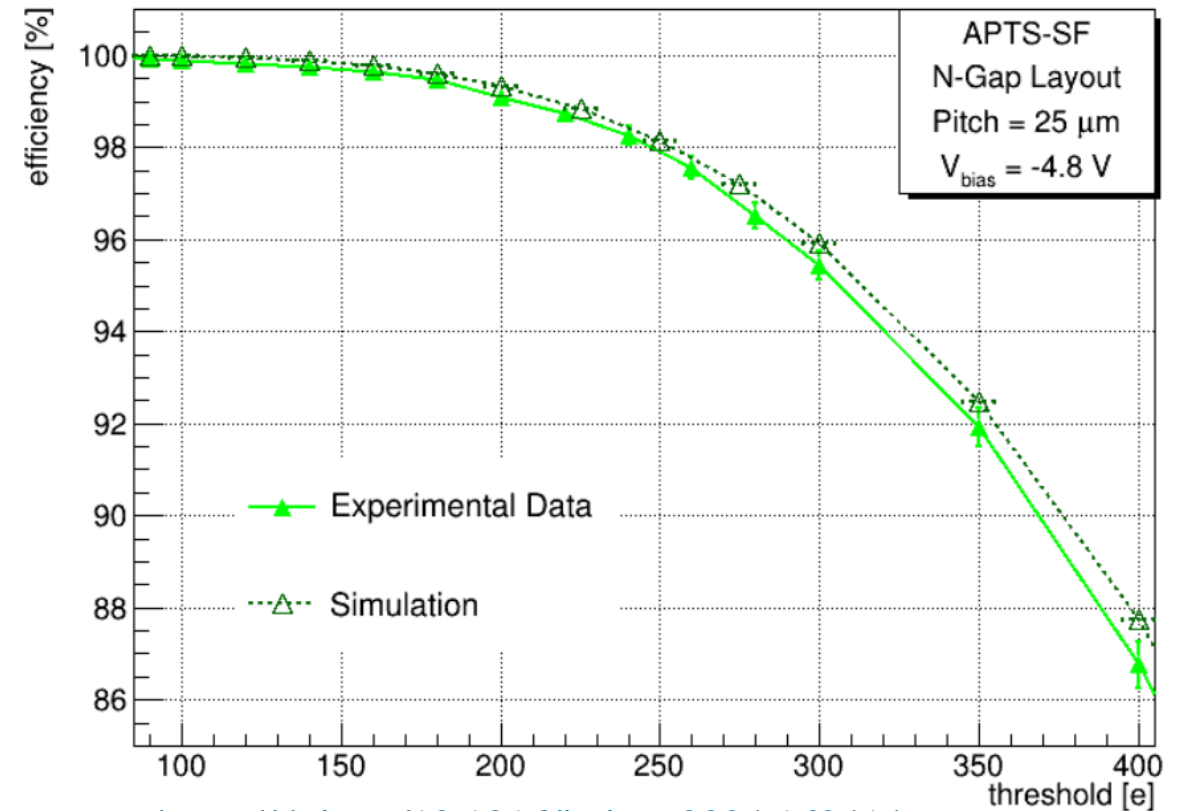
Conclusions and outlook

- Simulations are a **powerful tool** for sensor understanding and development

- A technology-independent approach using generic doping profiles has been developed for silicon sensor simulations; a **generic toolbox**, free from proprietary information

- Next steps for **simulations** in the Tangerine project:
  - Properly define the **uncertainties of the simulation results**, by varying parameters and quantifying their impacts
    - So far, error bars are purely statistical
  - **Compare to data** from testbeams carried out on test chips
    - This will allow for **validation of the predictive power** of the simulations

- Accurate simulations will **guide the way** to future sensor submissions
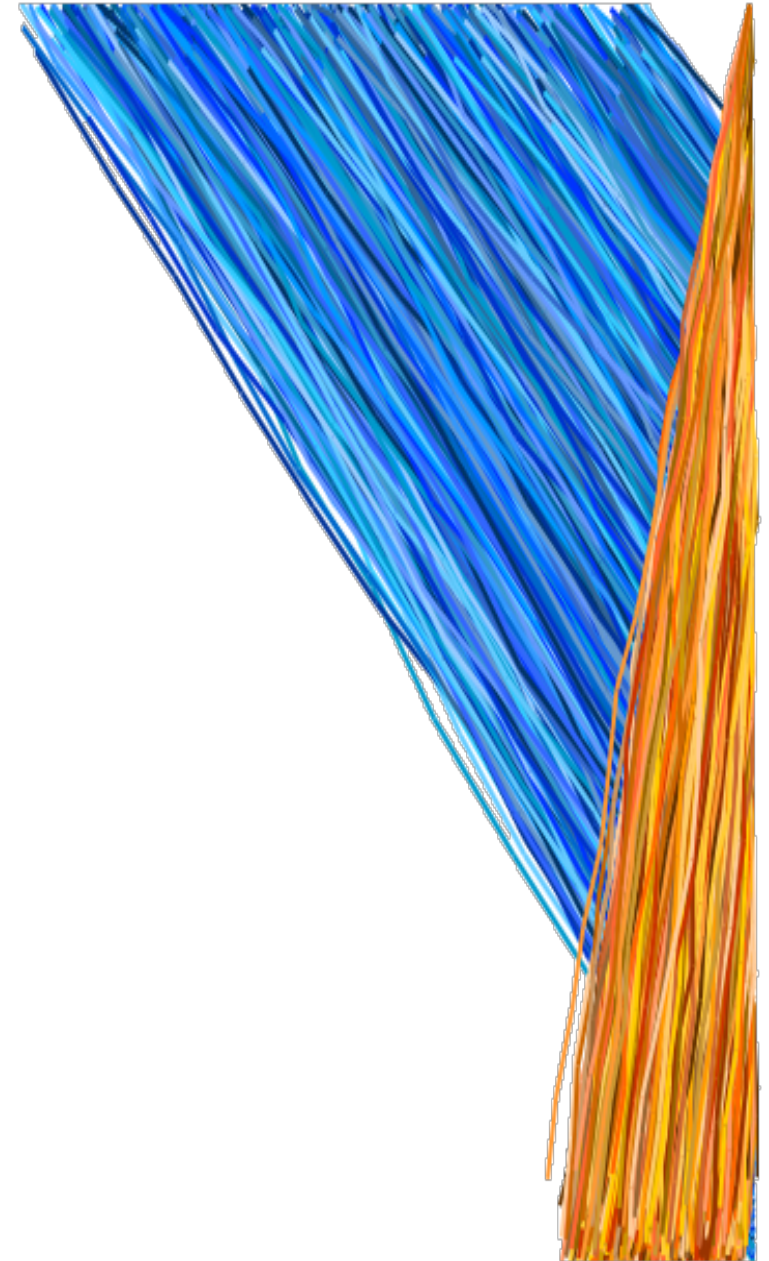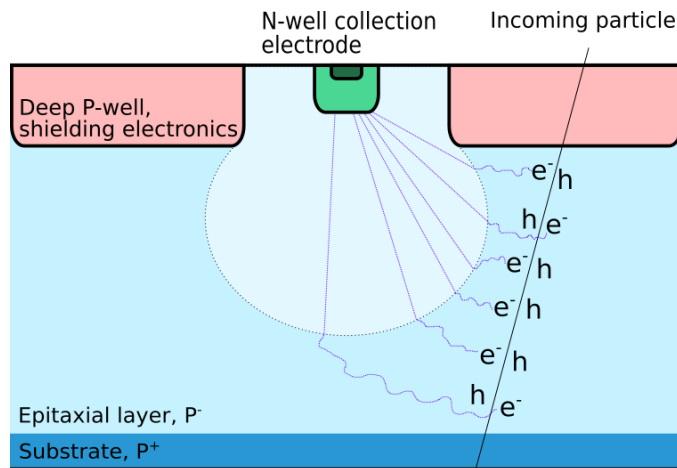
Backup slides

Rules followed in determining sensible sensor parameters

- The doping concentrations in the interfaces between different doping structures (n- and p-wells, epitaxial layer/substrate) should be diffused to avoid unphysical effects, such as abrupt changes in doping concentration and the corresponding electric field.

- The p-well must shield its content from the electric field in the active sensor area; the doping must thus be sufficient for it to only be depleted very near its boundaries.

- The charge carriers generated in the sensor volume have to reach the collection electrode.

- There should be no conductive channel between different biased structures, i.e. punch-through in the sensor should be avoided.

- The limitations on the operating voltages of the transistors in the readout electronics should be respected.

Sensor design

- The sensor design comprises both sensitive volume and electronics design

- For the sensitive volume design, there are three available layouts (all with a **small collection electrode**) originally designed for a 180 nm CMOS imaging process:

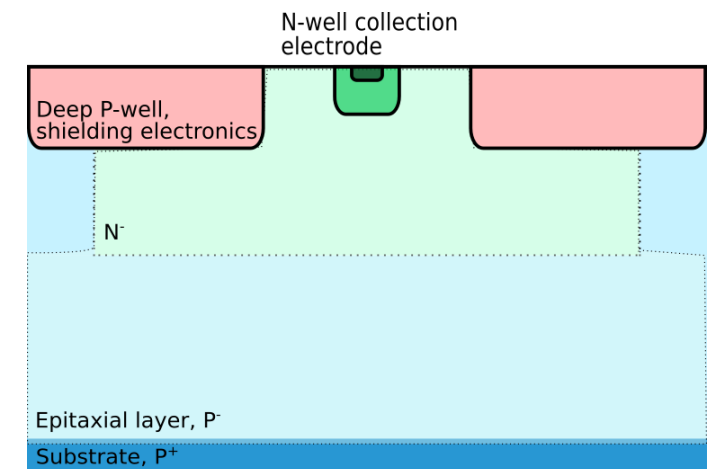|		
- Standard layout	- N-blanket layout	- N-gap layout
– ALPIDE-like	– Blanket layer of n-doped silicon, creating a **deep planar junction**	– Blanket n-layer **with gaps at pixel edges**

S. Senyukov et al. doi:10.1016/j.nima.2013.03.017
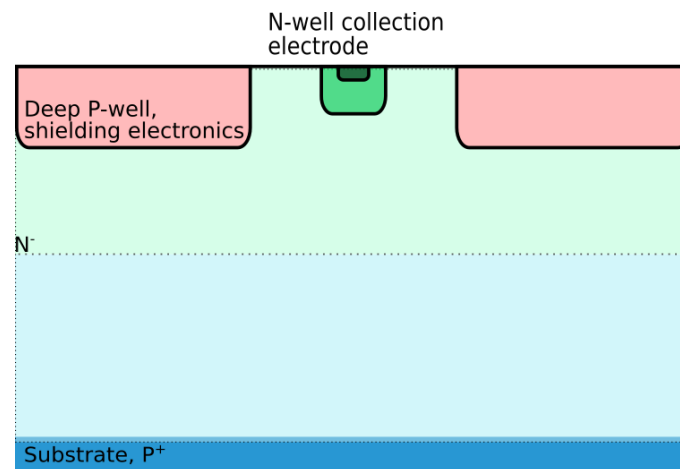
W. Snoeys et al. doi:10.1016/j.nima.2017.07.046

M. Münker et al 2019 JINST 14 C05013

Monte Carlo simulations using Allpix²

Impact of dopant diffusion simulation

- Linegraphs to demonstrate charge carrier movement

- Without simulated dopant diffusion, a **significant electric field appears** in the epitaxial layer-substrate interface

  - This is **unphysical**

- With simulated dopant diffusion (see slide 9), there is a **smooth transition region** rather than a step function

  - More natural, and provides a better match to data
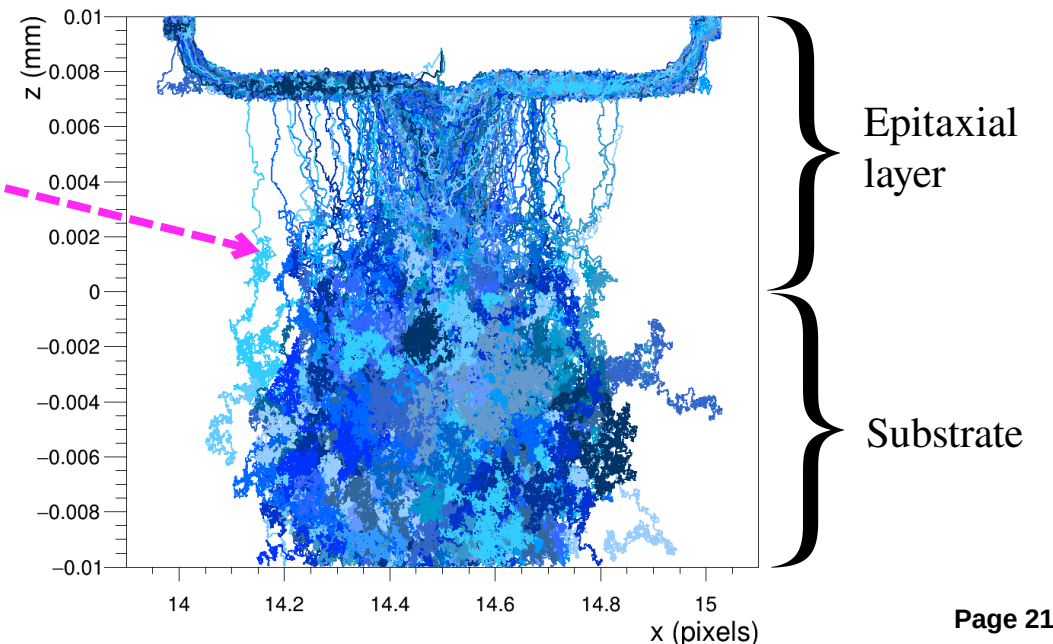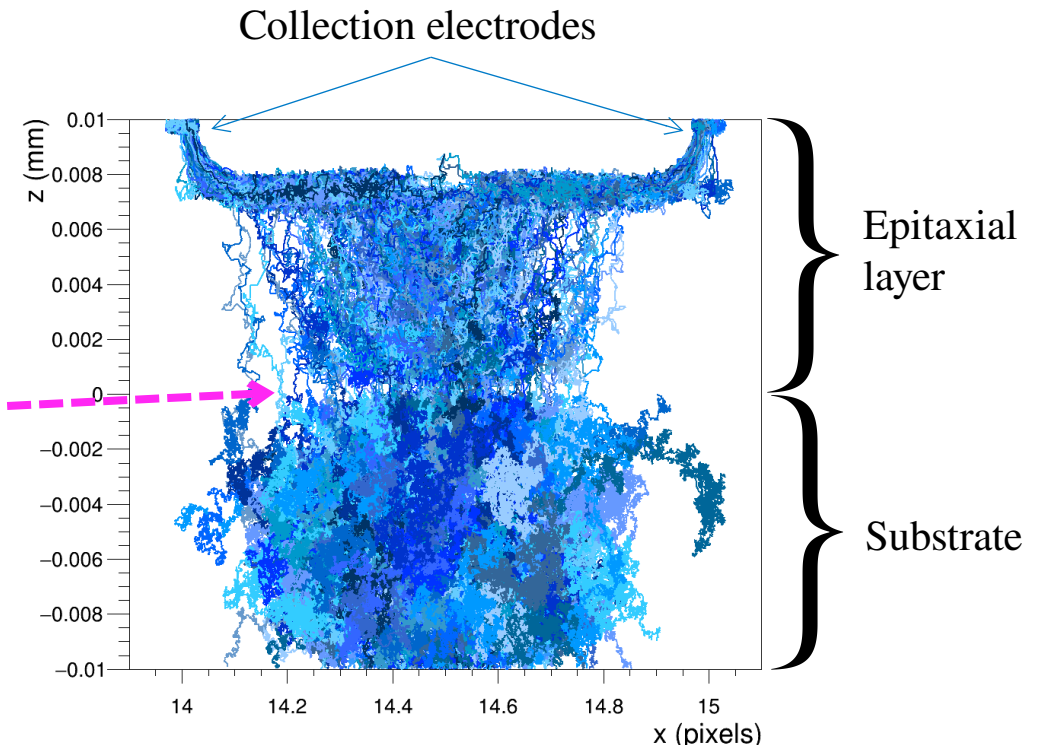
Transient simulations, comparing TCAD and Allpix²

- Generating weighting potentials for use in Allpix², from the electrostatic potentials from TCAD

  - Using Allpix² for the transient simulations gives a **lower computational cost**, and allows use of **Geant4 energy deposition**

- First step: compare Allpix² results to TCAD results

  - Allpix² results are the average of 10 000 events, TCAD is a single event

  - Same settings are used for charge carrier creation and mobility

  - Results in general agreement

- Allows for simulation of sensor **time response** and further **front-end electronics** simulations
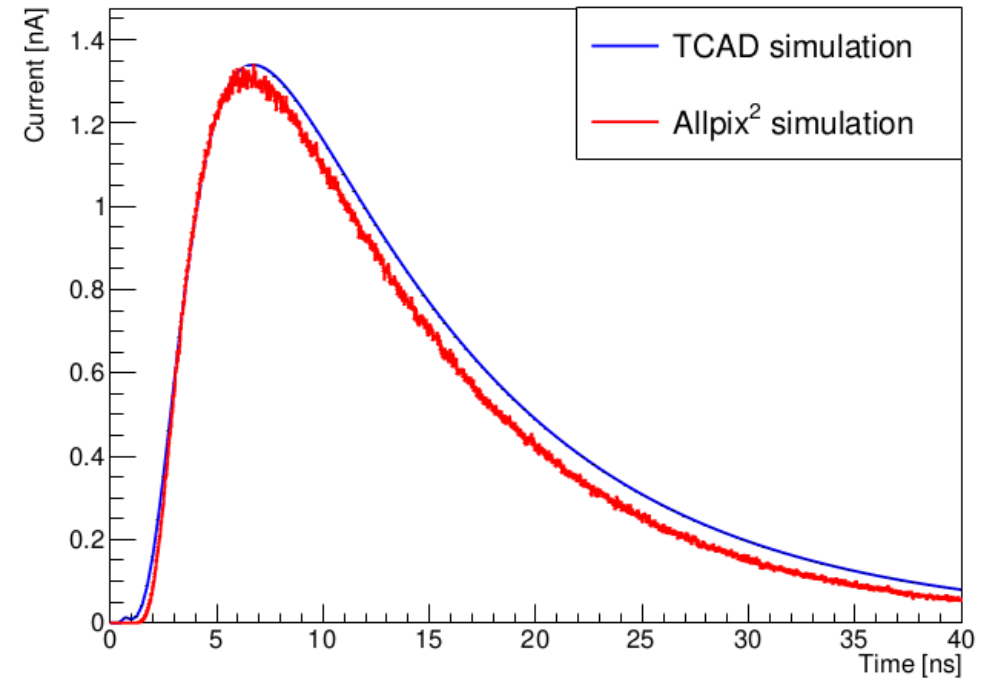

(a) *Standard* layout

Example observables for sensor characterisation

Cluster size

- **Number of pixels that register hits for a single incident particle** (charge sharing)

- This will depend on the position of the incident particle, but with a **large number of particles** a mean value can be found, as well as the cluster size versus hit position

- Varies with threshold value

Efficiency

- Denotes the **fraction of particles incident on the sensor that produce a signal in the sensor**

- Goes between 0 and 1
  - If all particles traversing the sensor produce a signal, the sensor is 100% efficient
  - Desirable to have **as high as possible**

- Strongly related to threshold value

- Can find mean efficiency across the sensor, and look at efficiency versus hit position

: Pixel registering hit

- - - : Particle track
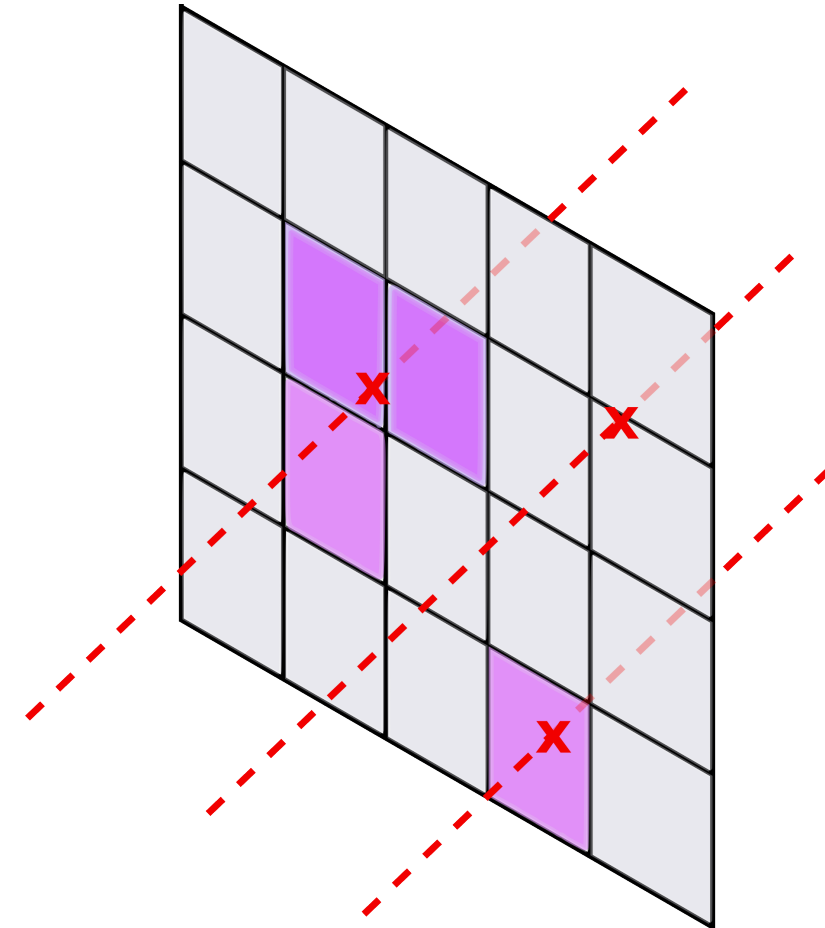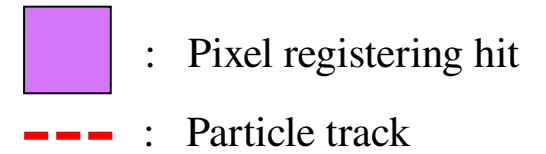
Monte Carlo simulations using Allpix²

Impact of mobility model

- Mobility model also impacts **final observables**

- High-statistics simulations allow extraction of observables such as cluster size, resolution, efficiency

- Figure shows **sensor efficiency vs detection threshold**, for two different mobility models

  - Simulation carried out with a DESY II-like beam of electrons

  - Each point corresponds to 500 000 events, so the statistical error bars are very small

- The doping-independent mobility model **over-estimates efficiency**, due to an excess of charge collected from the highly-doped substrate
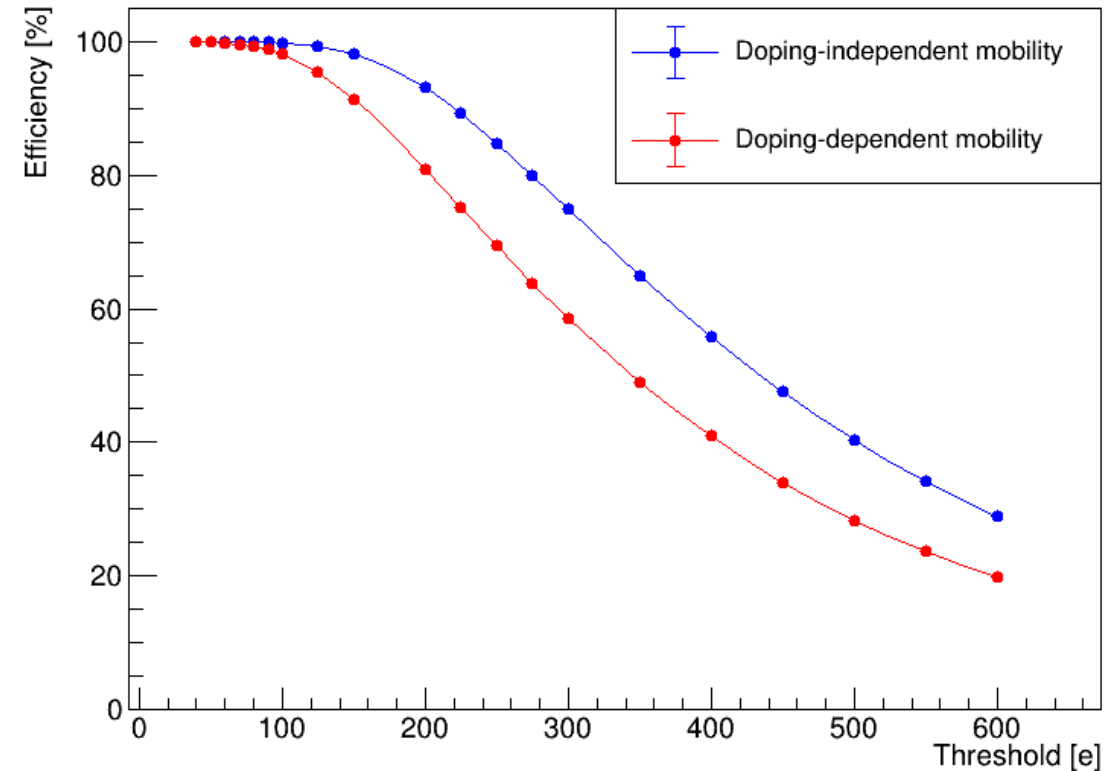

Sensor efficiency vs threshold for two different mobility models

Allpix² combined with TCAD - different pixel geometries ▢ ⬡

Example result from the [Tangerine project](#)

- Simulations allow for comparison of the performance of different sensor geometries

- A hexagonal layout leads to **reduced charge sharing in pixel corners** and a reduced distance from pixel boundary to pixel centre

  - May allow efficient operation at higher thresholds, and possibly better spatial resolution

- Tests have been performed comparing square pixels and hexagonal pixels, **maintaining the pixel area**

  - The space available for readout electronics thus remains the same per pixel

- Figure compares hexagonal pixels 18 μm corner-to-corner, and 15x15 μm² square pixels, in an ALPIDE-like layout
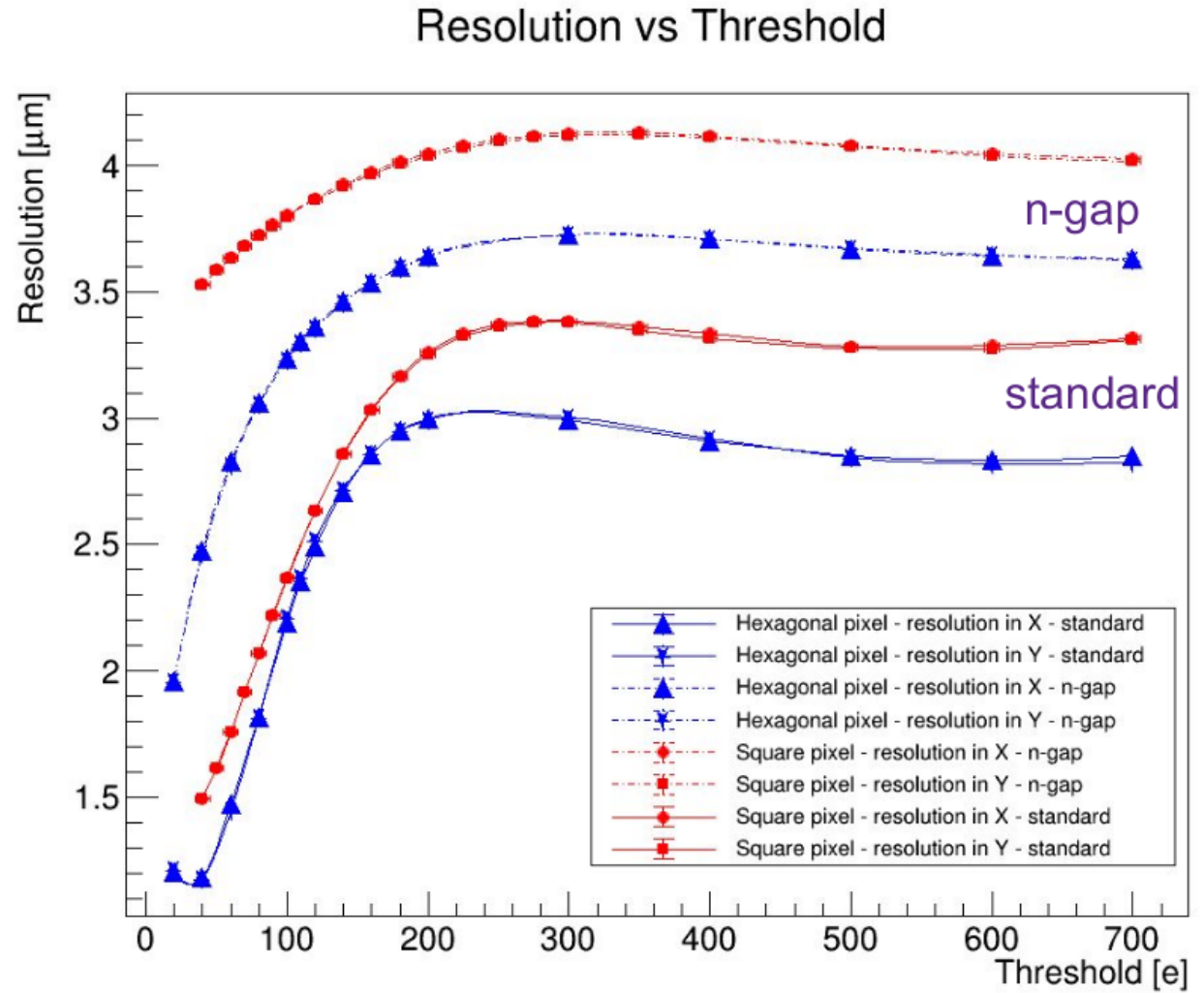
Resolution vs Threshold
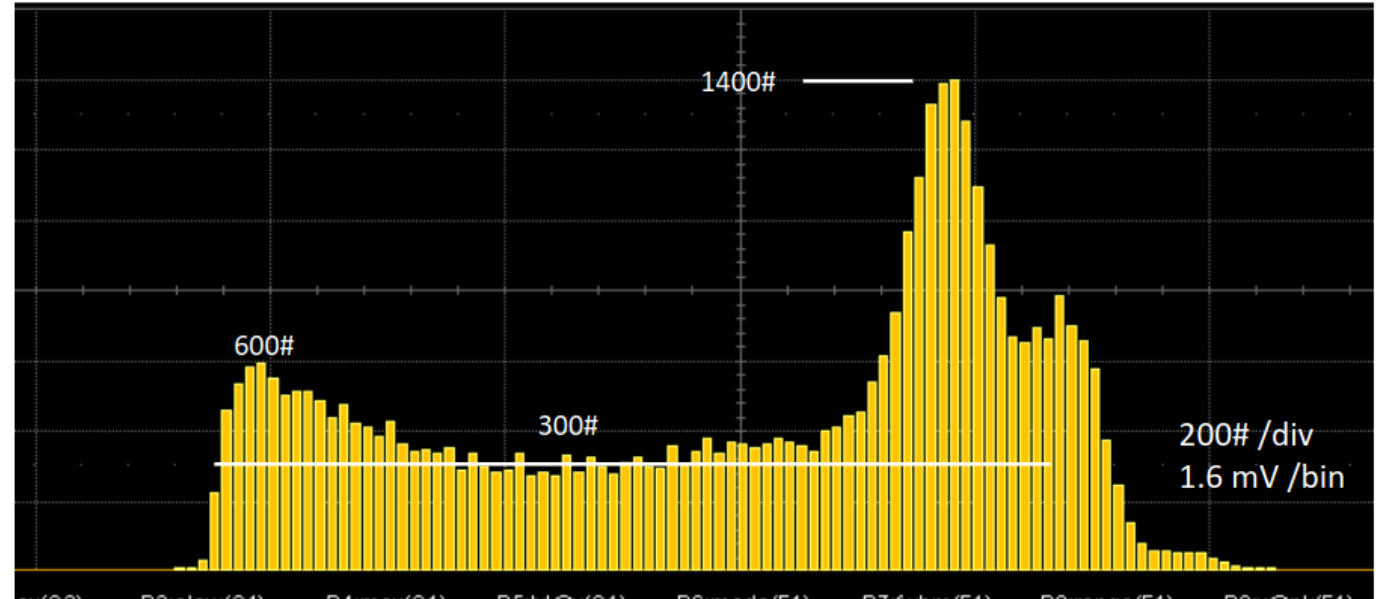
Allpix² combined with TCAD - Charge collection time of DESY ER1

Example result from the Tangerine project

- DESY ER1 prototype sensor

- 2x2 matrix with **rectangular pixels** of size 35x25 µm²

- Tests with **iron-55**
  - Signal amplitude results are **unexpected!**
  - Two-peak structure, but **not** K_α and K_β

- Theory: deposits far from pixel centre get **collected slowly**, so some charge **drains away before peaking**

- Higher Krummenacher current (i.e. faster return to baseline) leads to **two-peak structure** of single-energy x-ray
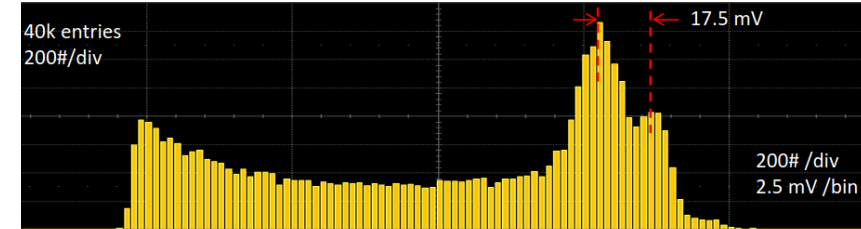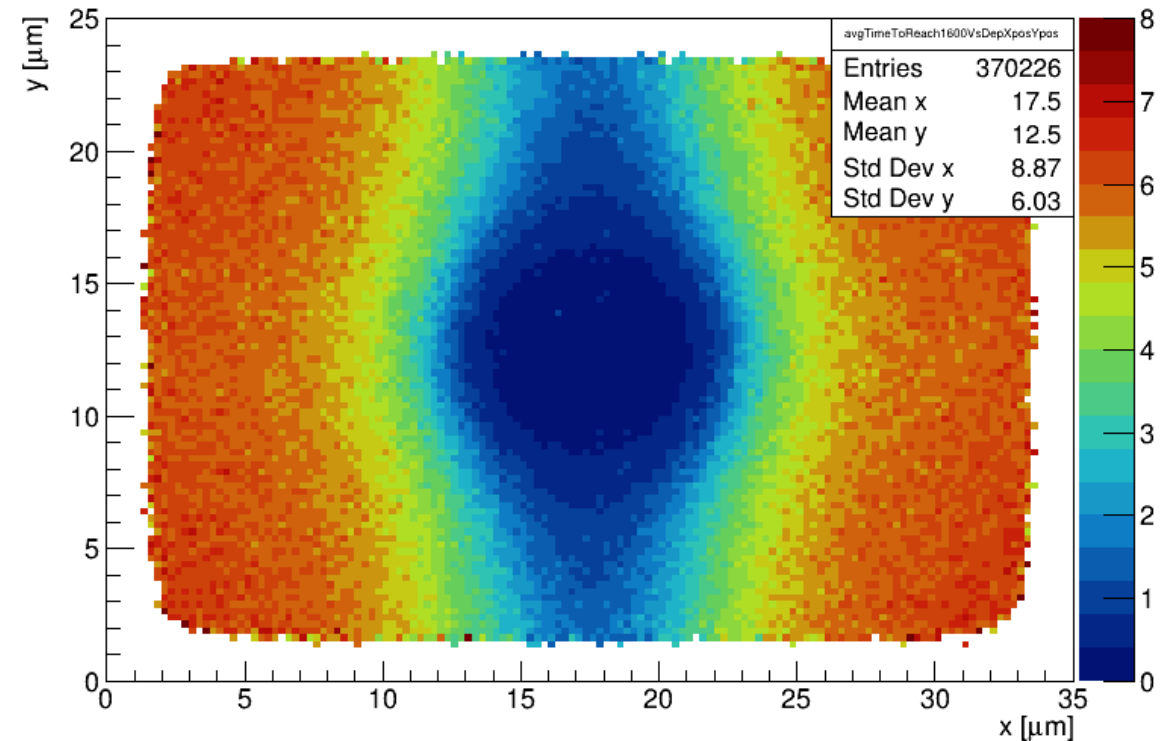
Amplitude histogram:

https://indico.desy.de/event/43834/contributions/167831

Allpix² combined with TCAD - Charge collection time of DESY ER1

Example result from the Tangerine project

- Charge deposition simulated over a full pixel, with 1640 electrons in each point

- Plot shows time taken to collect 1600 electrons

- There are **clear regions of different collection time**

- This can explain the two-peak structure seen in lab tests

  - Slower collection means that **more charge drains away** before peaking, leading to a **lower maximum amplitude**

Average time to reach 1600 electrons

avgTimeToReach1600VsDepXposYpos	
Entries	370226
Mean x	17.5
Mean y	12.5
Std Dev x	8.87
Std Dev y	6.03

Allpix² combined with TCAD - Charge collection time of DESY ER1

Example result from the Tangerine project

- Charge deposition simulated over a full pixel, with 1640 electrons in each point

- Plot shows time taken to collect 1600 electrons

- There are **clear regions of different collection time**

- This can explain the two-peak structure seen in lab tests

  - Slower collection means that **more charge drains away** before peaking, leading to a **lower maximum amplitude**
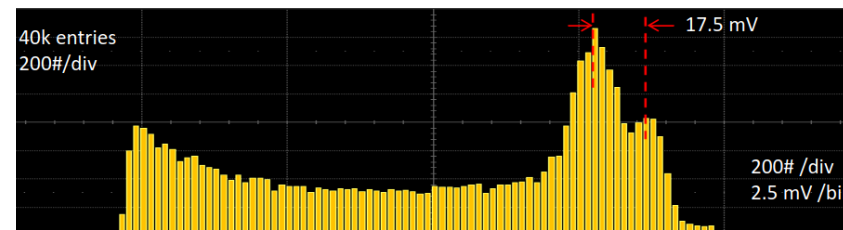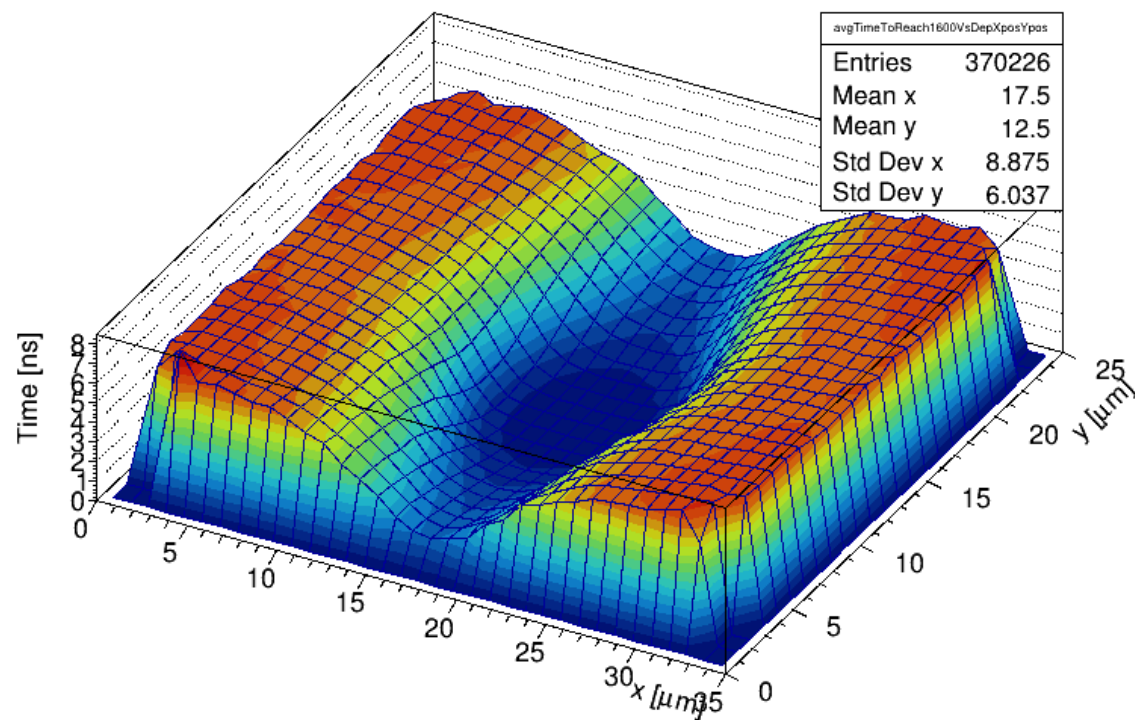

Average time to reach 1600 electrons

avgTimeToReach1600VsDepXposYpos	
Entries	370226
Mean x	17.5
Mean y	12.5
Std Dev x	8.875
Std Dev y	6.037

# Allpix² combined with TCAD - Charge collection time of DESY ER1

Example result from the Tangerine project

- Lateral electric field magnitude

- In x, we have **a region with low field** between gap and collection electrode

- This is also in y, but **much smaller due to the smaller distance** - we never go as low as in x

- This leads to overall faster charge collection, as charges are **constantly pushed** towards the collection electrode

- Simulations are a **powerful tool** for providing **understanding** of results

Lateral electric field at z=0.019000 mm
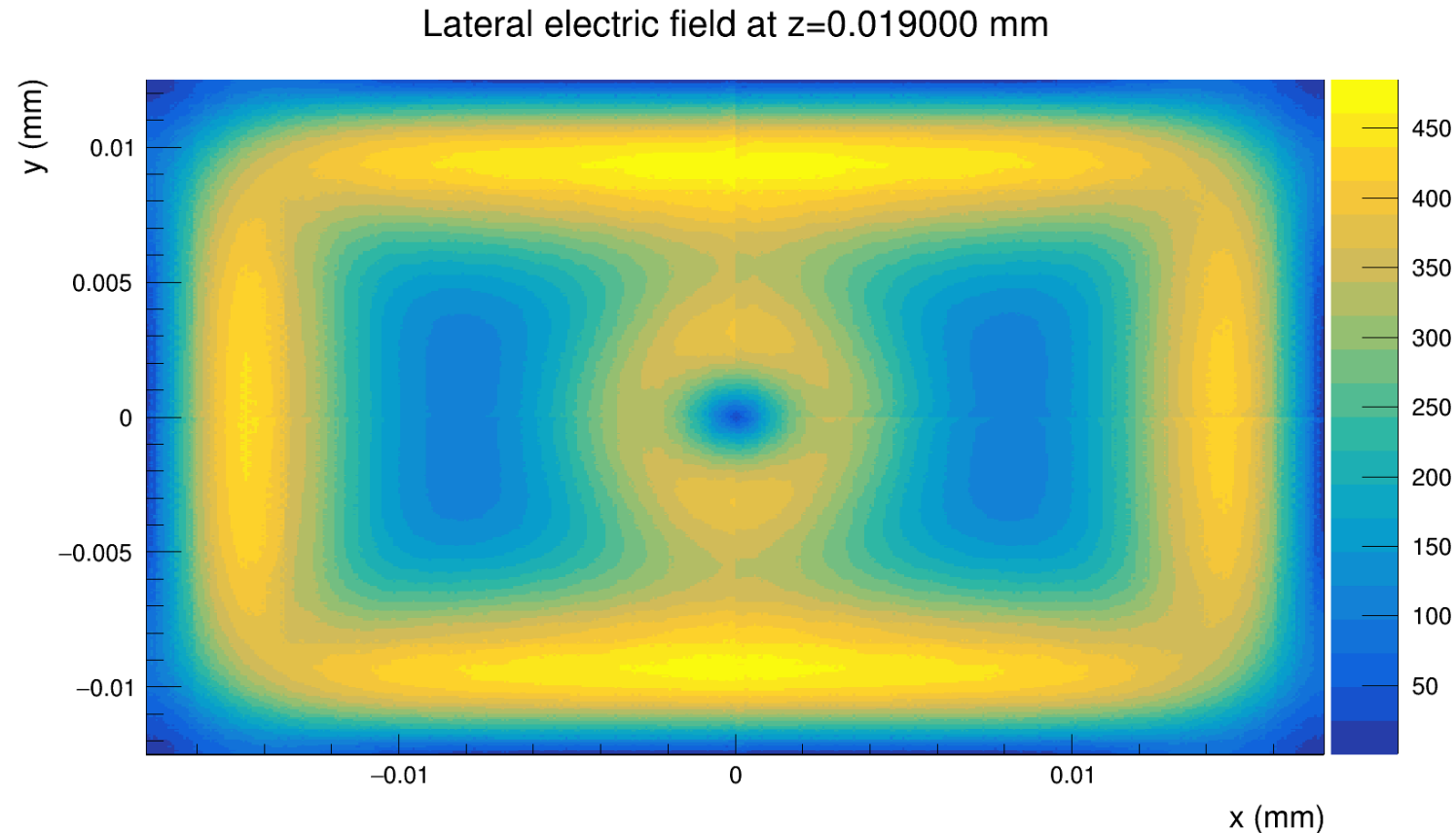
Transient simulations, comparing linear energy deposition to Geant4

- Using the n-blanket layout

- Each signal is the average of 10 000 events, incident in the pixel corner

- Geant4 energy deposition includes stochastic effects, while linear deposit generates 63 electron-hole pairs per μm

N-blanket layout, corner incidence
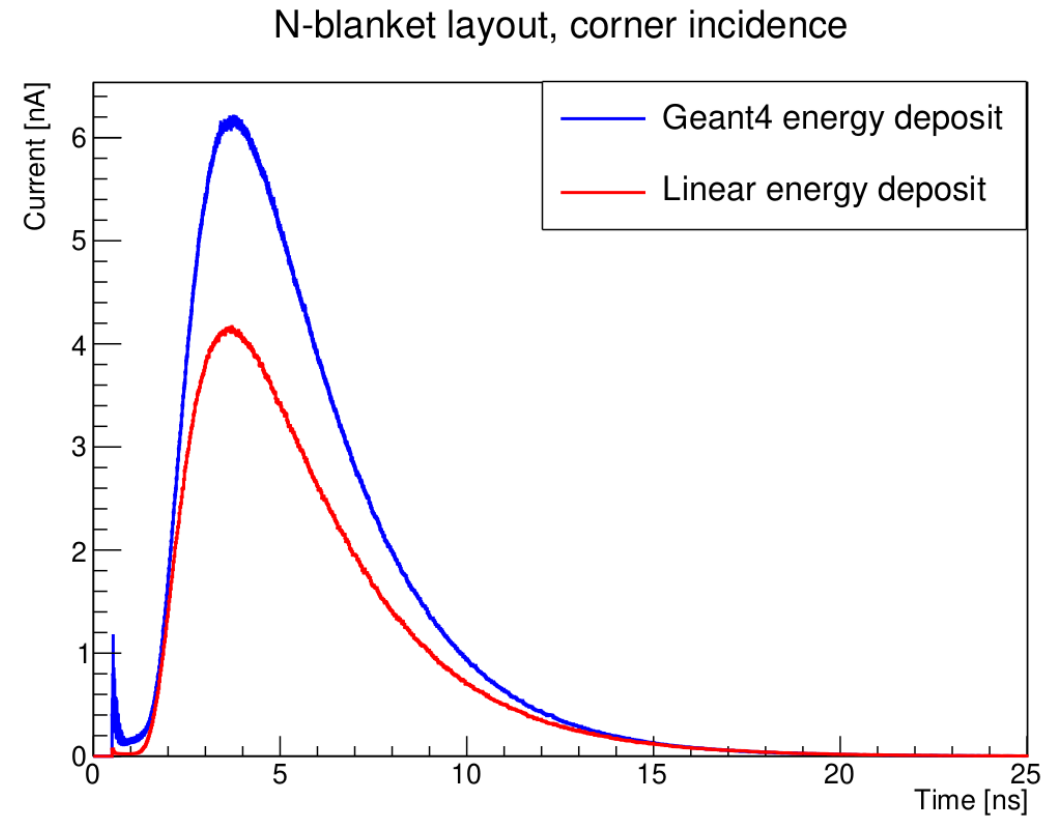
The Tangerine project: published references

- The Tangerine project: Development of high-resolution 65 nm silicon MAPS

  - https://doi.org/10.1016/j.nima.2022.167025

- Towards a new generation of Monolithic Active Pixel Sensors

  - https://doi.org/10.1016/j.nima.2022.167821

- Developing a Monolithic Silicon Sensor in a 65 nm CMOS Imaging Technology for Future Lepton Collider Vertex Detectors

  - https://doi.org/10.1109/NSS/MIC44845.2022.10398964

- Simulations and performance studies of a MAPS in 65 nm CMOS imaging technology

  - https://doi.org/10.1016/j.nima.2024.169414