Simulating monolithic active pixel sensors

A technology-independent approach using generic doping profiles

H. Wennlöf for the Tangerine collaboration



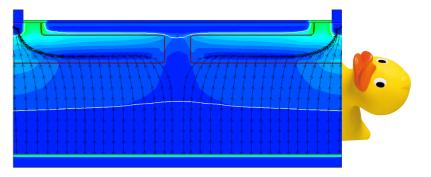
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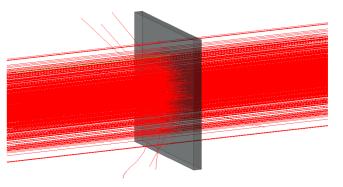
The Tangerine collaboration at DESY: A. Chauhan, M. Del Rio Viera, J. Dilg, D. Eckstein, F. Feindt, I.-M. Gregor, Y. He, K. Hansen, L. Huth, S. Lachnit, L. Mendes, B. Mulyanto, D. Rastorguev, C. Reckleben, S. Ruiz Daza, J. Schlaadt, P. Schütze, A. Simancas, S. Spannagel, M. Stanitzki, A. Velyka, G. Vignola,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

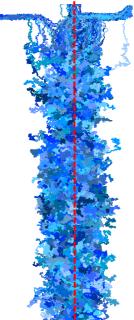
Outline

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



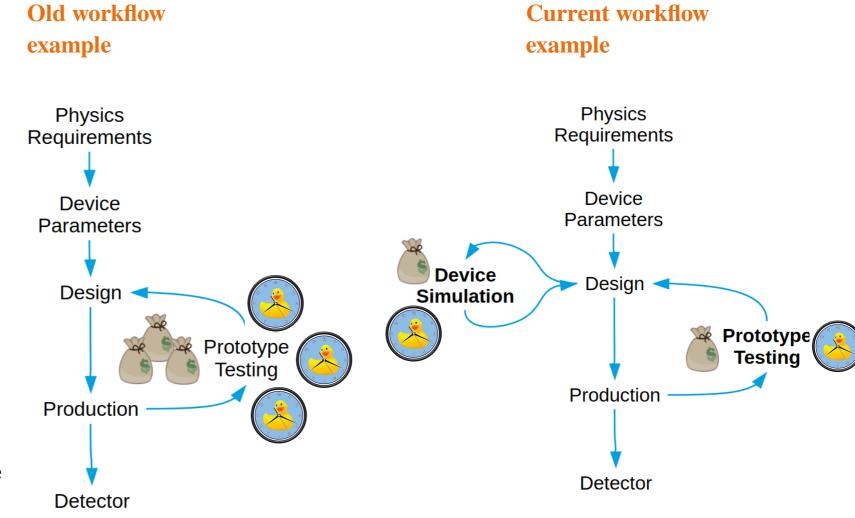






Motivation for simulations

- A way to **understand and predict** sensor behaviour
- Computing power is relatively cheap nowadays
 - Simulations are cheaper and faster than prototype production
- Simulations also help in providing a deeper understanding of measurement results
- A combination of detailed simulations and prototype testing can be used to efficiently guide the way in sensor developments

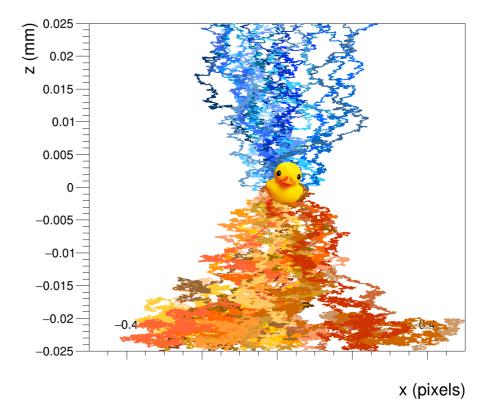


Figures by A. Simancas, <u>BTTB10</u>

DESY.

Silicon sensor simulations

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

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DESY.

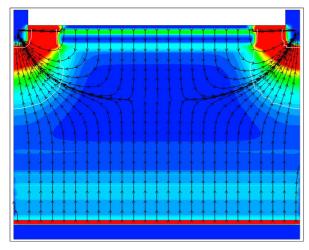
Tools used in the simulation approach

Sentaurus TCAD



Technology Computer-Aided Design

- Models semiconductor devices using finite element methods
- Calculates realistic and accurate electric fields and potentials from doping concentrations



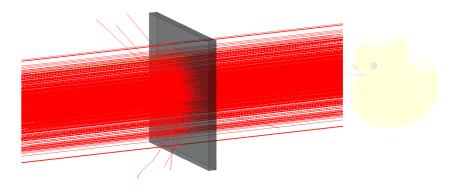
Example electric field in TCAD



Allpix Squared: a Monte Carlo simulation framework for semiconductor detectors

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

- 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

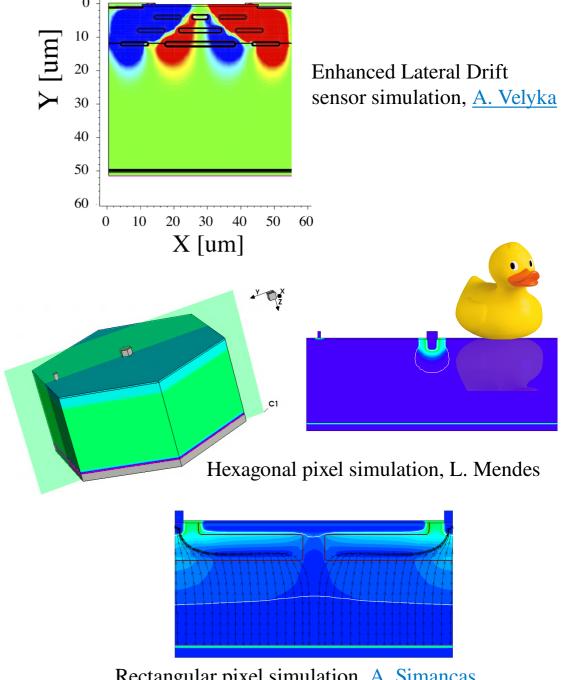


Particle beam passing through a single sensor in Allpix²

TCAD

Technology computer-aided design

- 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



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 3.0.3 released on December 14th 2023
- <u>User workshop</u> 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"
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beam_direction = 0 0 1
[ProjectionPropagation]
[SimpleTransfer]
[DefaultDigitizer]
```

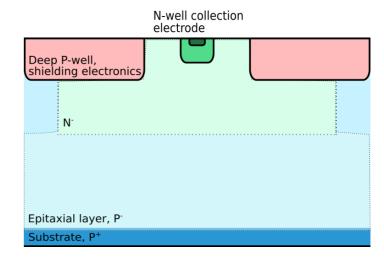
Minimal simulation configuration example

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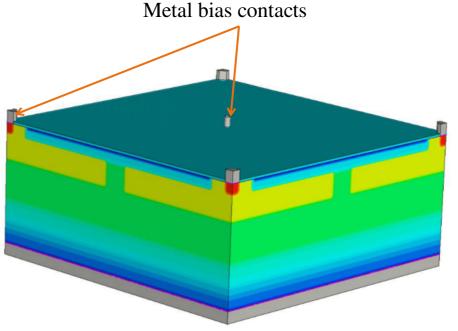
Silicon simulation layout and assumptions

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
- 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



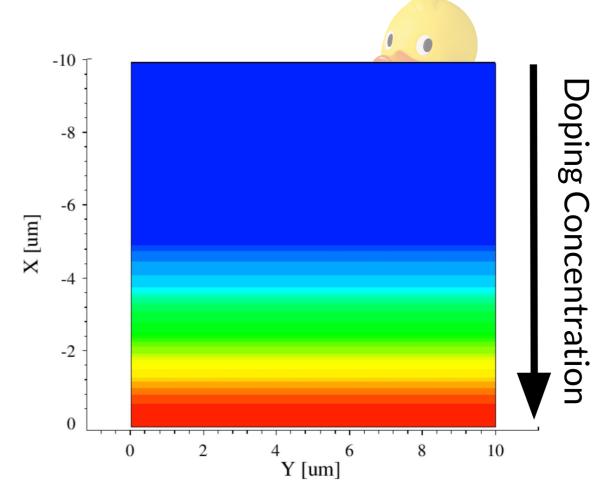
"N-gap layout", M. Münker et al 2019 JINST 14 C0501



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

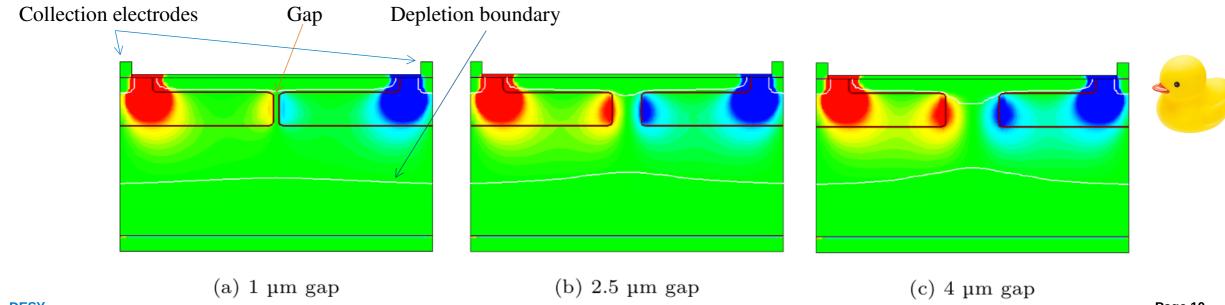


Process simulation result, showing dopant diffusion between substrate and epitaxial layer

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

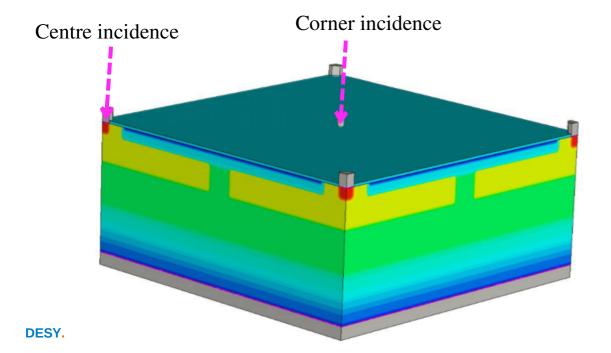


DESY.

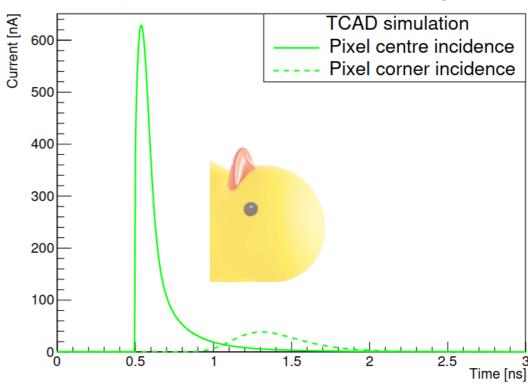
Finite element method simulations using TCAD

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



Square pixels, 20x20 μm^2 , n-gap layout



Transient pulses for pixel centre and corner incidence

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- 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

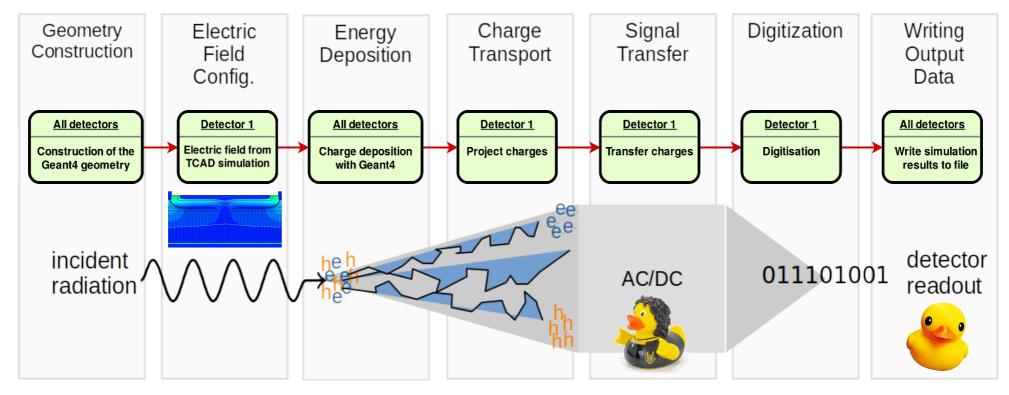
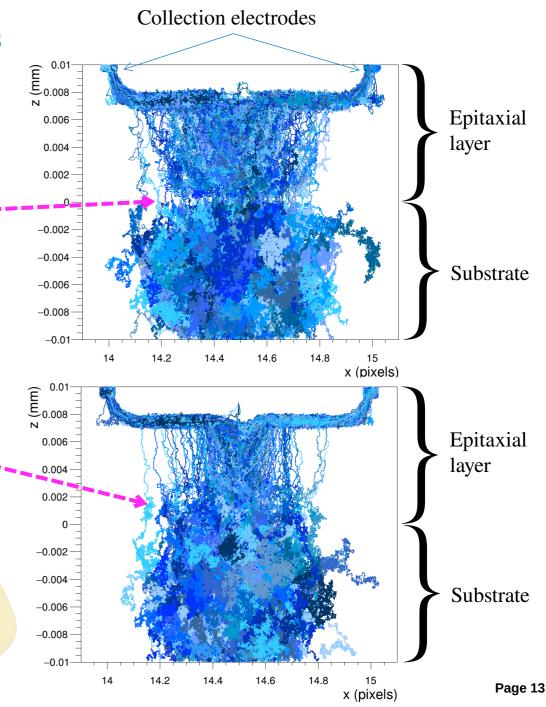


Figure from S. Spannagel, BTTB10, and A. Simancas, 4th Allpix Squared User Workshop

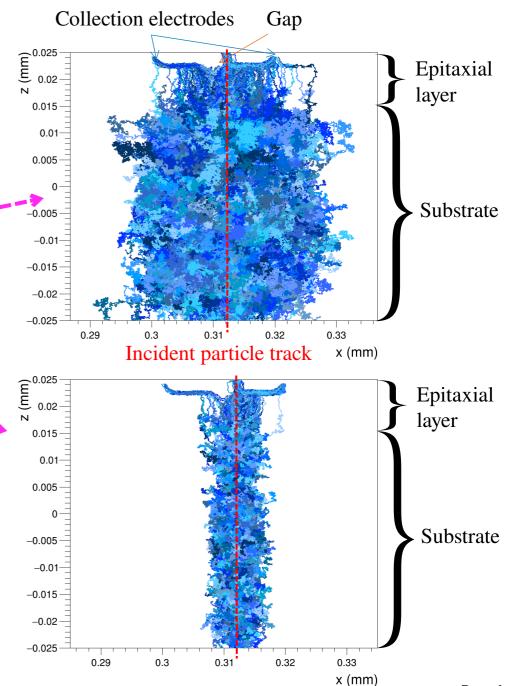
Impact of dopant diffusion simulation

- 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



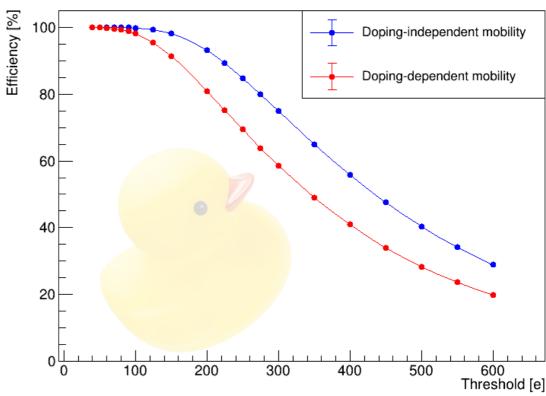
Impact of mobility model

- 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 dopingdependent
 - 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



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 **overestimates efficiency**, due to an excess of charge collected from the highly-doped substrate



Sensor efficiency vs threshold for two different mobility models

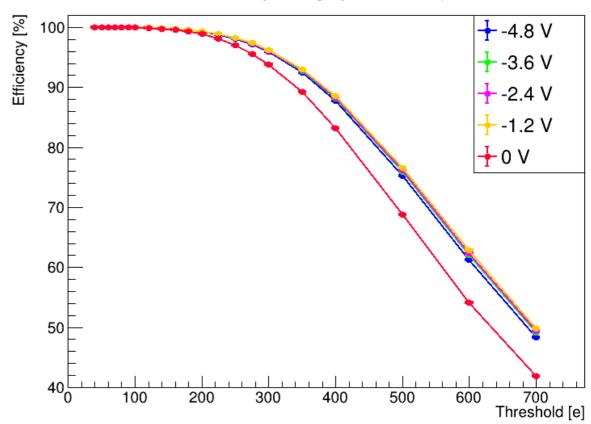
Allpix² combined with TCAD

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







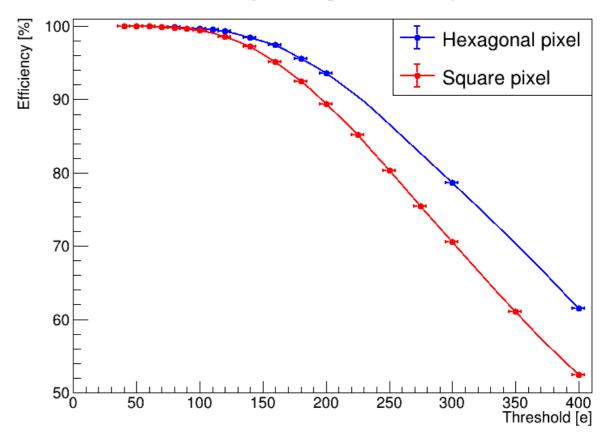
Allpix² combined with TCAD - different pixel geometries \Box



Example result from the Tangerine project

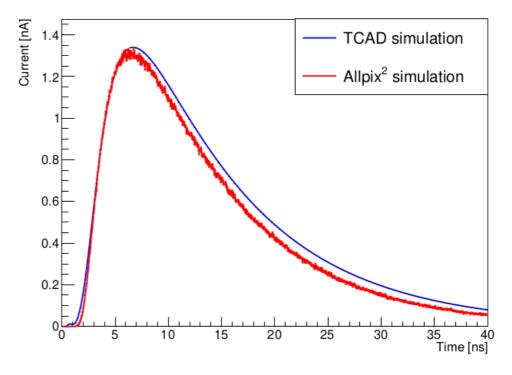
- Simulations allow for comparison of the performance of different sensor geometries
- A hexagonal layout leads to reduced charge sharing in pixel corners and a reduced distance from pixel boundary to pixel centre
 - Allows efficient operation at higher thresholds, and possibly better spatial resolution
- 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 the standard layout (ALPIDE-like)

Efficiency, hexagonal and square



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

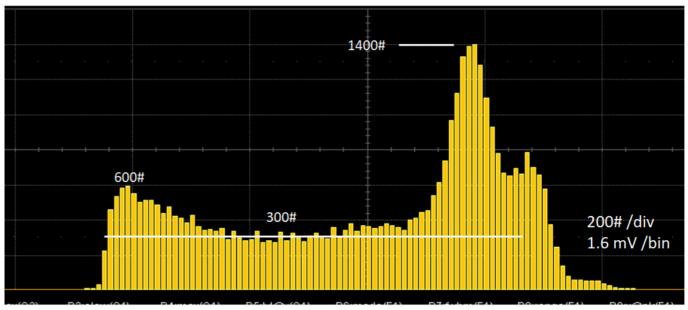


(a) Standard layout

Example 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

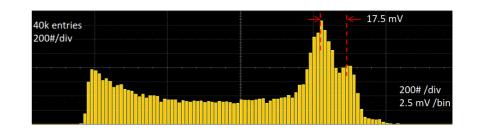
Amplitude histogram:



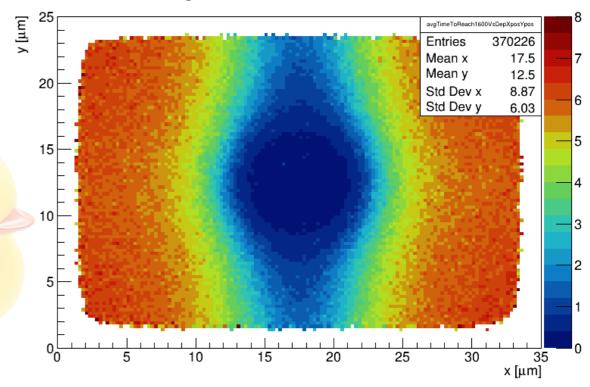
https://indico.desy.de/event/43834/contributions/167831

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**

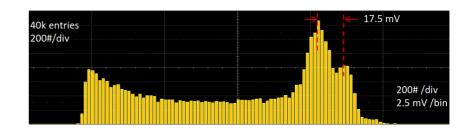


Average time to reach 1600 electrons

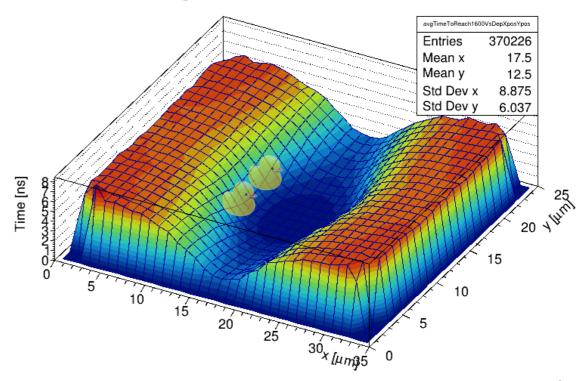


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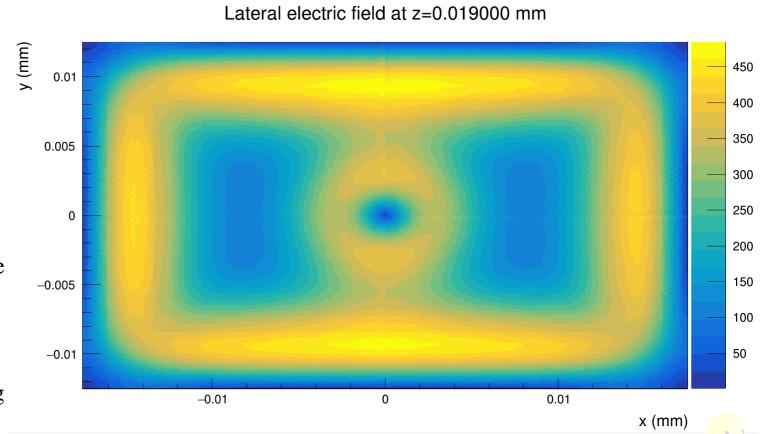
Average time to reach 1600 electrons



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

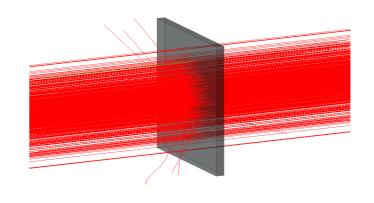
 Simulations are a powerful tool for providing understanding of results

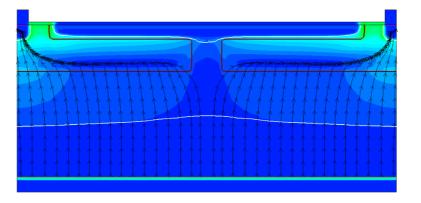


Simulations compared to data

Does the procedure actually work?









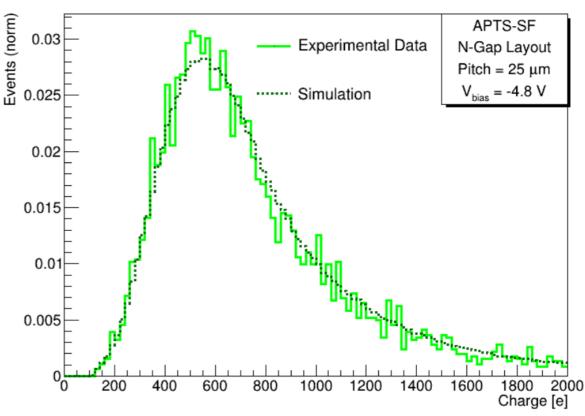
Allpix² combined with TCAD - Preliminary comparison to data

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 μ m² pixel size
 - 4x4 pixel matrix
 - -4.8 V bias voltage
- The trend between simulations and data **matches well**



Cluster charge distribution



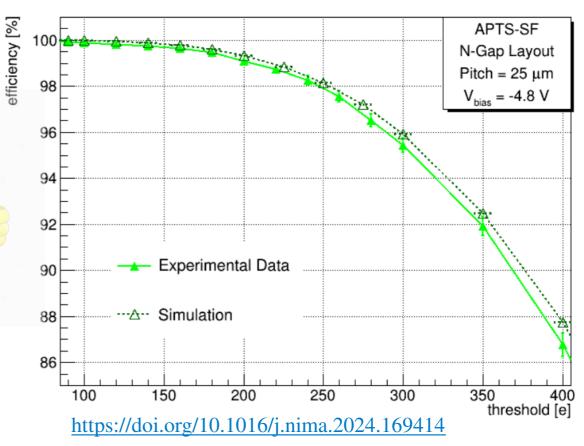
https://doi.org/10.1016/j.nima.2024.169414

Allpix² combined with TCAD - Preliminary comparison to data

Example result from the Tangerine project

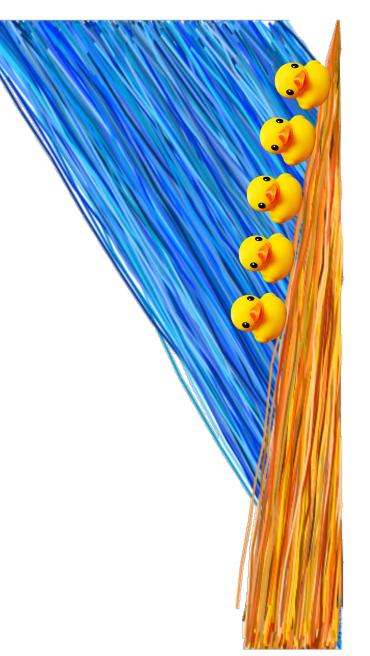
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- Results from the "Analog Pixel Test Structure" (APTS)
 - N-gap layout
 - 25x25 μ m² pixel size
 - 4x4 pixel matrix
 - -4.8 V bias voltage
- The trend between simulations and data matches well
 - Error bars on the simulated results are purely statistical here
- In conclusion, the developed **simulation procedure works well**, without any proprietary information

Mean efficiency vs threshold



Conclusions and outlook

- Simulations are a **ducking good 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
 - A paper describing it will be submitted soon
- 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

42 ducks in total



Rules followed in determining sensible sensor parameters

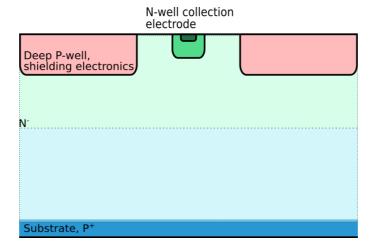
- The doping concentrations in the interfaces between different doping structures (n- and p-wells, epitaxial layer/substrate) should be diffused to avoid unphysical effects, such as abrupt changes in doping concentration and the corresponding electric field.
- The p-well must shield its content from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

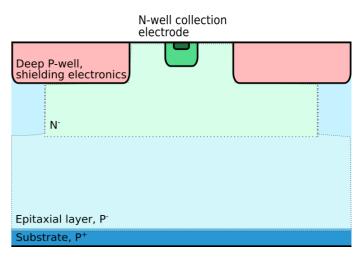
S. Senyukov et al. doi:10.1016/j.nima.2013.03.017

- N-blanket layout
 - Blanket layer of n-doped silicon, creating a deep planar junction



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

- N-gap layout
 - Blanket n-layer with gaps at pixel edges



M. Münker et al 2019 JINST 14 C05013

DESY.

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

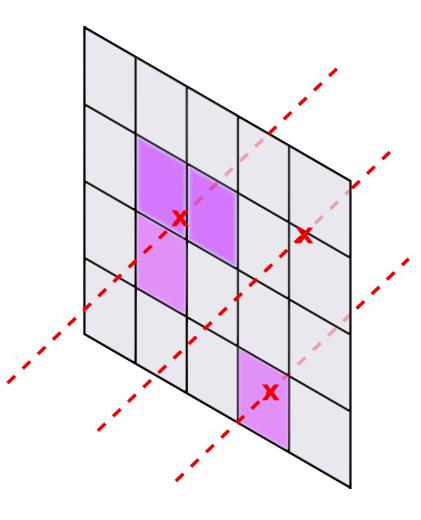
Efficiency

- 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

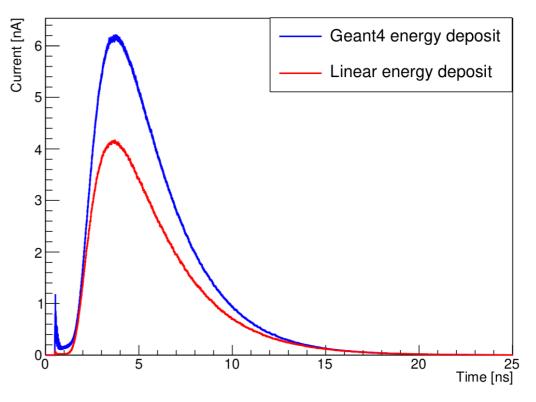
--- : Particle track



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

