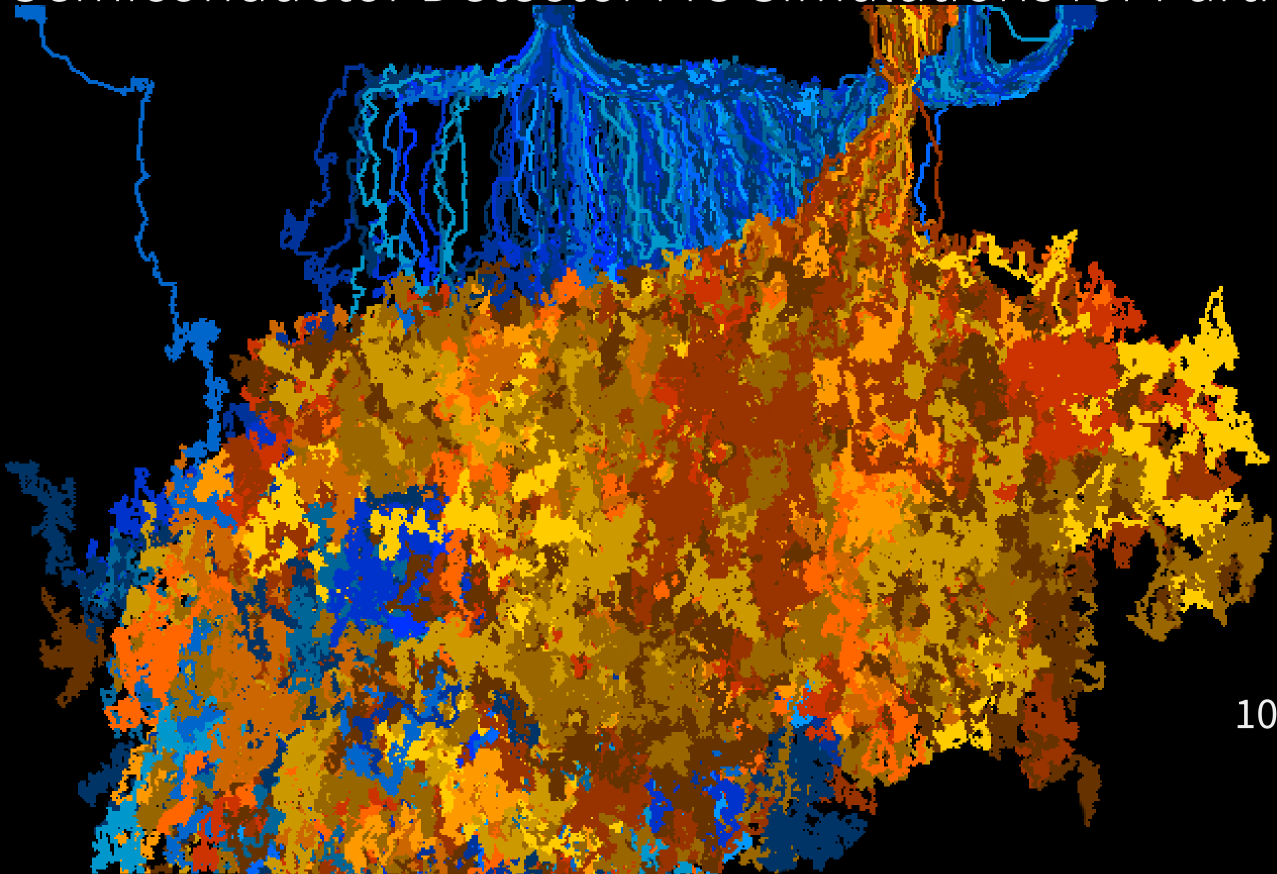
cern.ch/allpix-squared

Allpix Squared

Semiconductor Detector MC Simulations for Particle Physics and Beyond



Simon Spannagel, DESY
for the Allpix Squared Authors

10th PIXEL Workshop, Santa Fe, NM
15 December 2022

Mohamed Moanis Ali, GSOC2019 Student
Mathieu Benoit, ORNL
Thomas Billoud, Université de Montréal
Tobias Bisanz, CERN
Marco Bomben, Université de Paris
Koen van den Brandt, Nikhef
Carsten Daniel Burgard, DESY
Maximilian Felix Caspar, DESY
Liejian Chen, IHEP Beijing
Dominik Dannheim, CERN
Manuel Alejandro Del Rio Viera, DESY
Katharina Dort, University of Gießen
Neal Gauvin, Université de Genève
Lennart Huth, DESY
Daniel Hynds, University of Oxford
Francisco-Jose Iguaz-Gutierrez, Synchrotron SOLEIL
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Moritz Kiehn, Université de Genève
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Nashad Rahman, The Ohio State University
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Daniil Rastorguev, DESY
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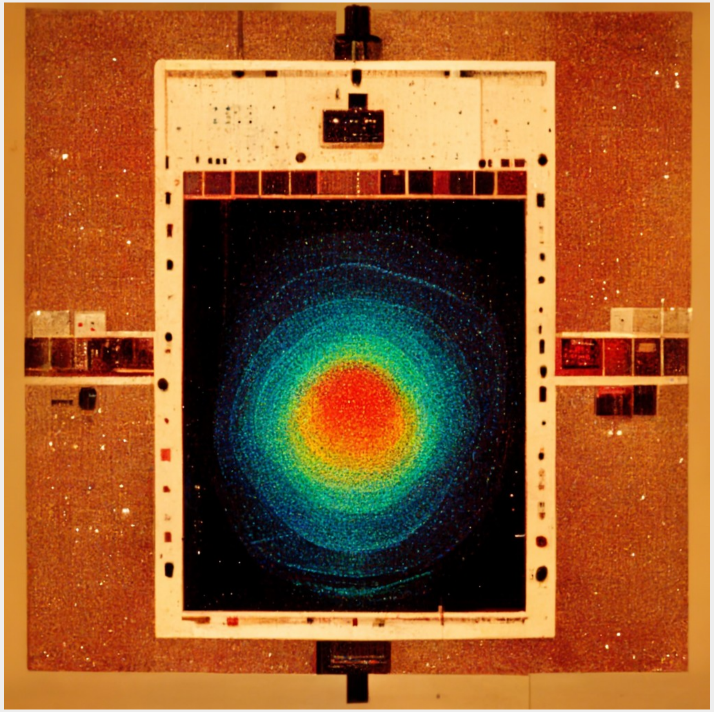
Mateus Vicente Barreto Pinto, Université de Genève
Håkan Wennlöf, DESY
Andy Wharton, Lancaster University
Morag Williams, University of Glasgow
Koen Wolters

Monte Carlo Simulations of Semiconductor Detectors

- Using Monte Carlo methods to describe detector response is not new
- Creation & proliferation of many different codes for detector simulation:
  - Experiment-specific
  - Specialized on specific detectors
  - Inclusion only of effects relevant to that one simulation
  - Written as part of a PhD thesis, abandoned afterwards

- **Wanted:**
  flexible, tested & supported MC simulation software…



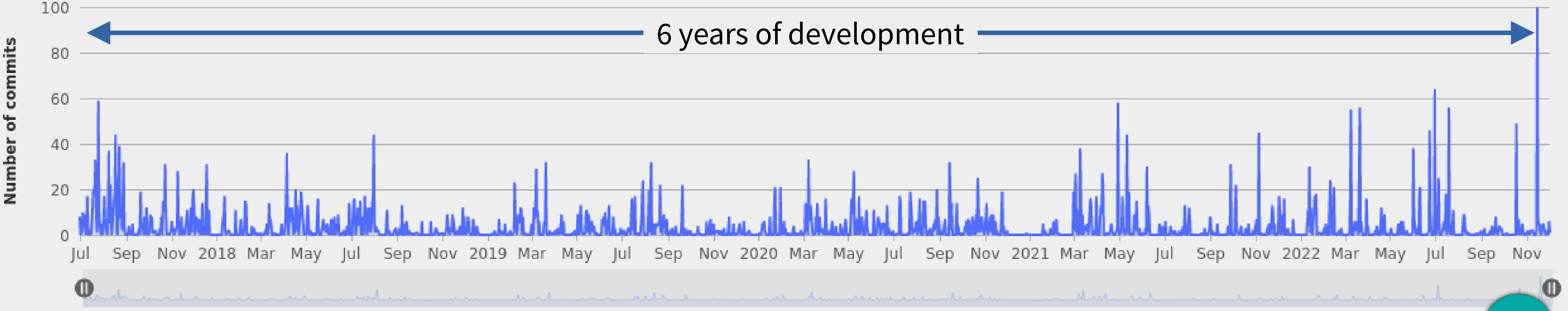
Midjourney,
`/image a silicon pixel detector measuring high-energetic particles`

The Allpix^2 Framework

- Development of new framework started within **CLICdp Collaboration**
- Now 6 years of development with
  - 44 releases, current version 2.3.3
  - 3 user workshops
  - > 50 code contributors

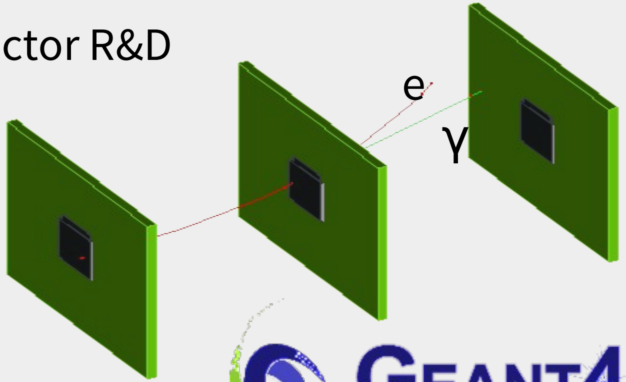
Development based on four principles:

I. Integration of Existing Toolkits
II. Well-Tested & Validated Algorithms
III. Low Entry Barrier for New Users
IV. Clean & Maintainable Code



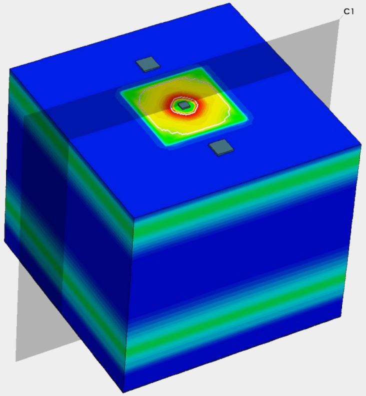
I. Integration of Existing Toolkits

Many very powerful tools developed and employed over decades of detector R&D
Leverage their capabilities by providing interfaces for their integration



Geant4 – simulating interactions of particles passing through matter

- Detailed simulation of many interactions & processes
- Cumbersome to use for beginners, complexity often overwhelming at first
- Provide abstraction layer to auto-generate models and run simulation



TCAD – solving Poisson's equation using finite element methods

- Detailed understanding of field configuration, sensor behavior
- Tools & knowledge widely spread in community
- Provide possibility to import results to complement MC simulations

II. Well-Tested & Validated Algorithms

Simulations provide insights into physical processes – but only if they model them correctly!

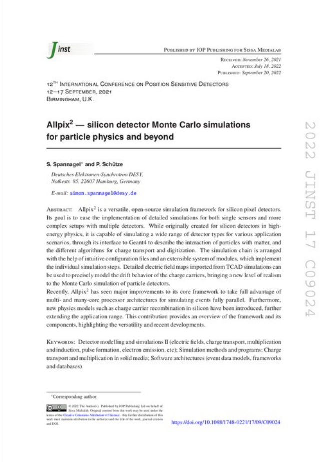
- Validation of algorithms is a crucial and time-consuming process
- User workshops for exchange of the community, discussions, planning…

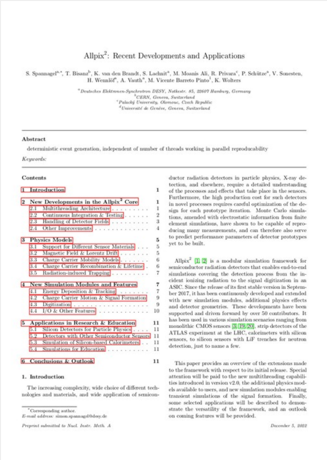
- Validating as much as possible against data
- Publishing reference studies including full simulation configuration used
- Providing automated tests for every new feature


NIMA 901 (2018) 164 – 172
doi:10.1016/j.nima.2018.06.020


NIMA 964 (2020) 163784
doi:10.1016/j.nima.2020.163784


NIMA 1031 (2022) 166491
doi:10.1016/j.nima.2022.166491

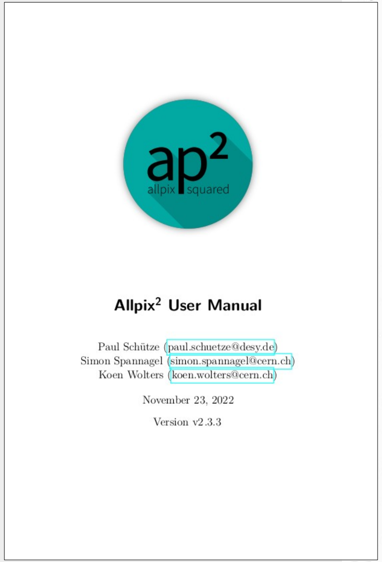

JINST 17 (2022) C09024
doi:10.1088/1748-0221/17/09/C09024


In preparation…

III. Low Entry Barrier for New Users

Simulation frameworks often very complex:
code complexity, lack of documentation, physics

- Allpix Squared attempts to facilitate quick starts:
  - Extensive documentation / user manual
  - Public forum for help & exchange
  - Human-readable configuration files
  - Support for physical units
  - No coding or code-reading required



Allpix^2 User Manual

Paul Schütze (paul.schuetze@desy.de)
Simon Spannagel (simon.spannagel@cern.ch)
Koen Wolters (koen.wolters@cern.ch)

November 23, 2022

Version v2.3.3

```
[AllPix]
log_level = "INFO"
number_of_events = 500000
detectors_file = "telescope.conf"

[GeometryBuilderGeant4]
world_material = "air"

[DepositionGeant4]
physics_list = FTFP_BERT_LIV
particle_type = "Pi+"
number_of_particles = 1
beam_energy = 120GeV
# ...

[ElectricFieldReader]
model="linear"
bias_voltage=150V
depletion_voltage=50V

[GenericPropagation]
temperature = 293K
charge_per_step = 10
spatial_precision = 0.0025um
timestep_max = 0.5ns

[SimpleTransfer]
```

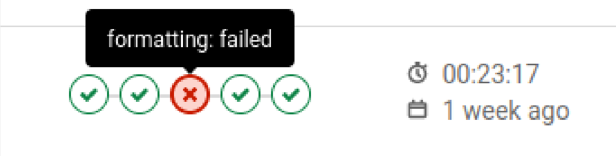
- Successfully used e.g. in university education, summer schools, …

Bonn-Cologne Graduate School
of Physics and Astronomy

EDIT-2020
Excellence in Detector and Instrumentation Technologies
School for Young Researchers

IV. Clean & Maintainable Code

Collaborative software development requires well-defined procedures –
Otherwise quickly becomes unmaintainable



formatting: failed

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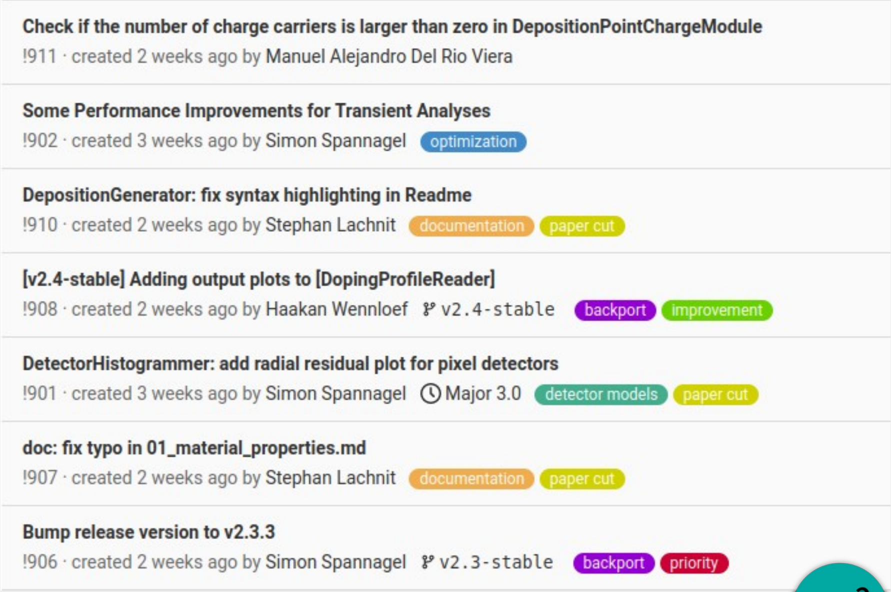
1 week ago

Allpix Squared implements *best practices* for software development

- Permissive MIT open-source license
- Semantic versioning (major.feature.patch)
- Extensive code reviews via merge requests
- Strict enforcement of coding conventions & formatting
- Regular static code analysis
- Following C++17 Standards



Check if the number of charge carriers is larger than zero in DepositionPointChargeModule
!911 · created 2 weeks ago by Manuel Alejandro Del Rio Viera

Some Performance Improvements for Transient Analyses
!902 · created 3 weeks ago by Simon Spannagel optimization

DepositionGenerator: fix syntax highlighting in Readme
!910 · created 2 weeks ago by Stephan Lachnit documentation paper cut

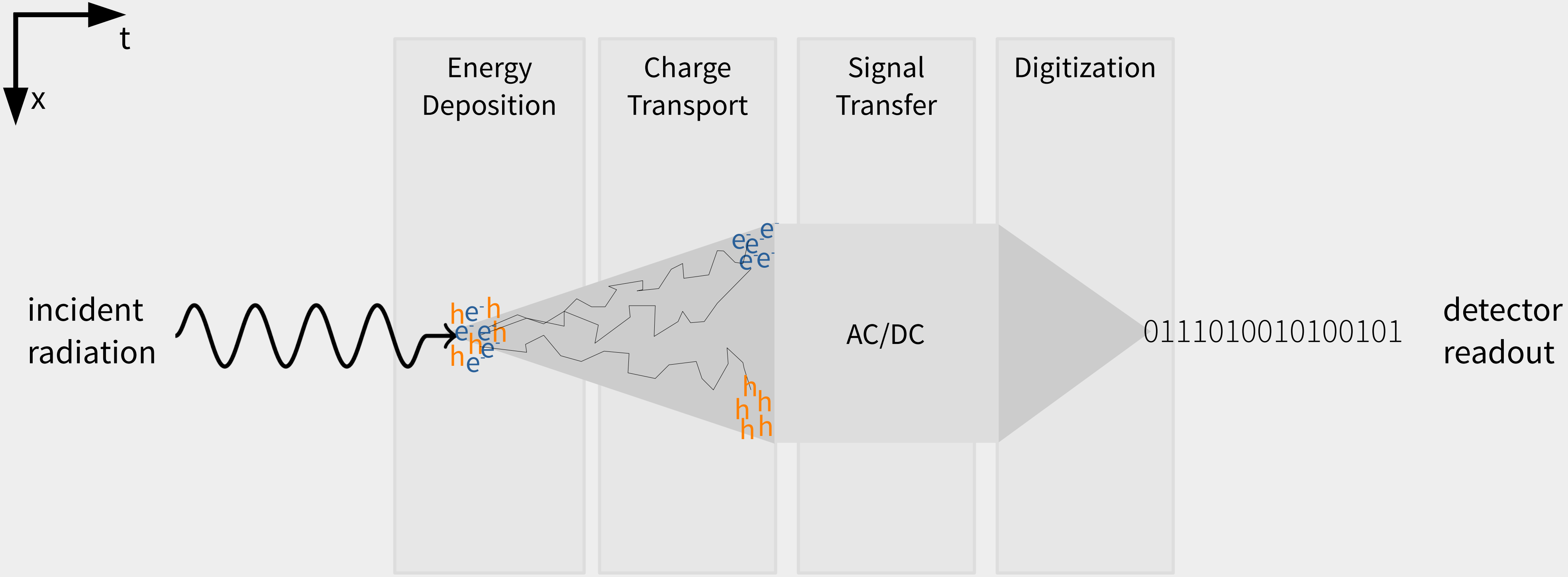
[v2.4-stable] Adding output plots to [DopingProfileReader]
!908 · created 2 weeks ago by Haakan Wennloef `v2.4-stable` backport improvement

DetectorHistogrammer: add radial residual plot for pixel detectors
!901 · created 3 weeks ago by Simon Spannagel Major 3.0 detector models paper cut

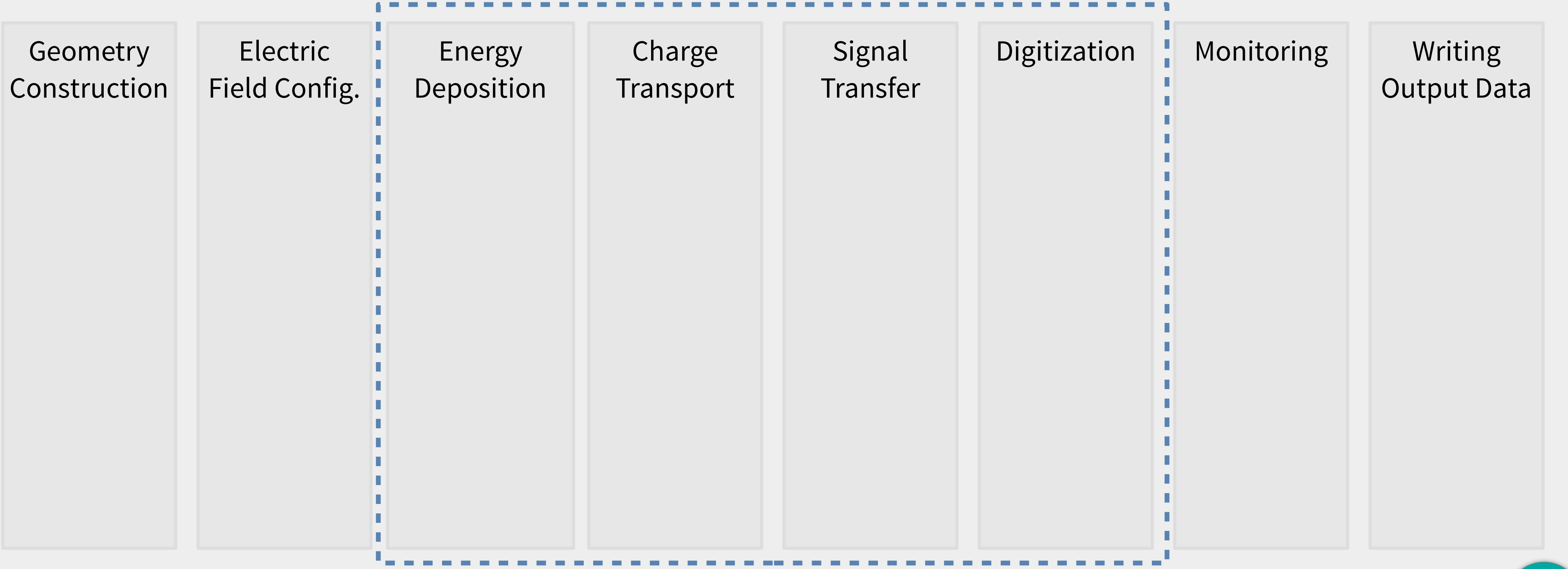
doc: fix typo in 01_material_properties.md
!907 · created 2 weeks ago by Stephan Lachnit documentation paper cut

Bump release version to v2.3.3
!906 · created 2 weeks ago by Simon Spannagel `v2.3-stable` backport priority

Particle Detection with Semiconductor Detectors



The Simulation Chain



Geometry Construction

Electric Field Config.

Energy Deposition

Charge Transport

Signal Transfer

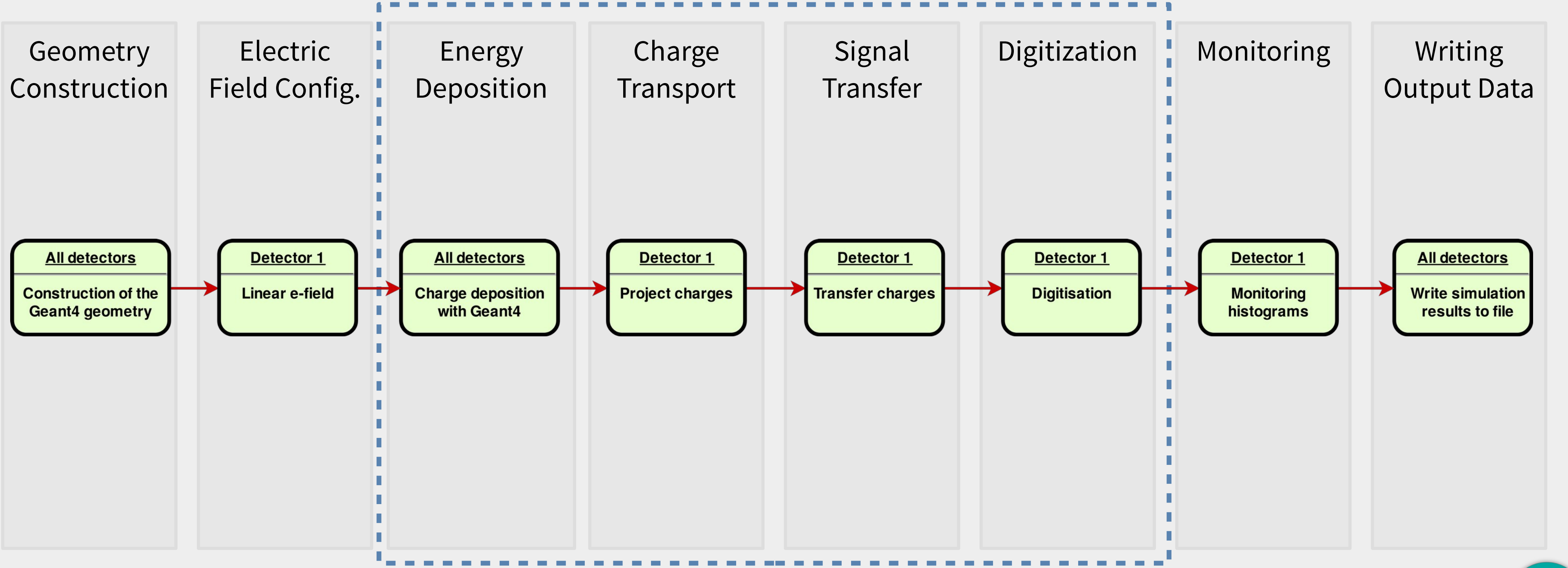
Digitization

Monitoring

Writing Output Data

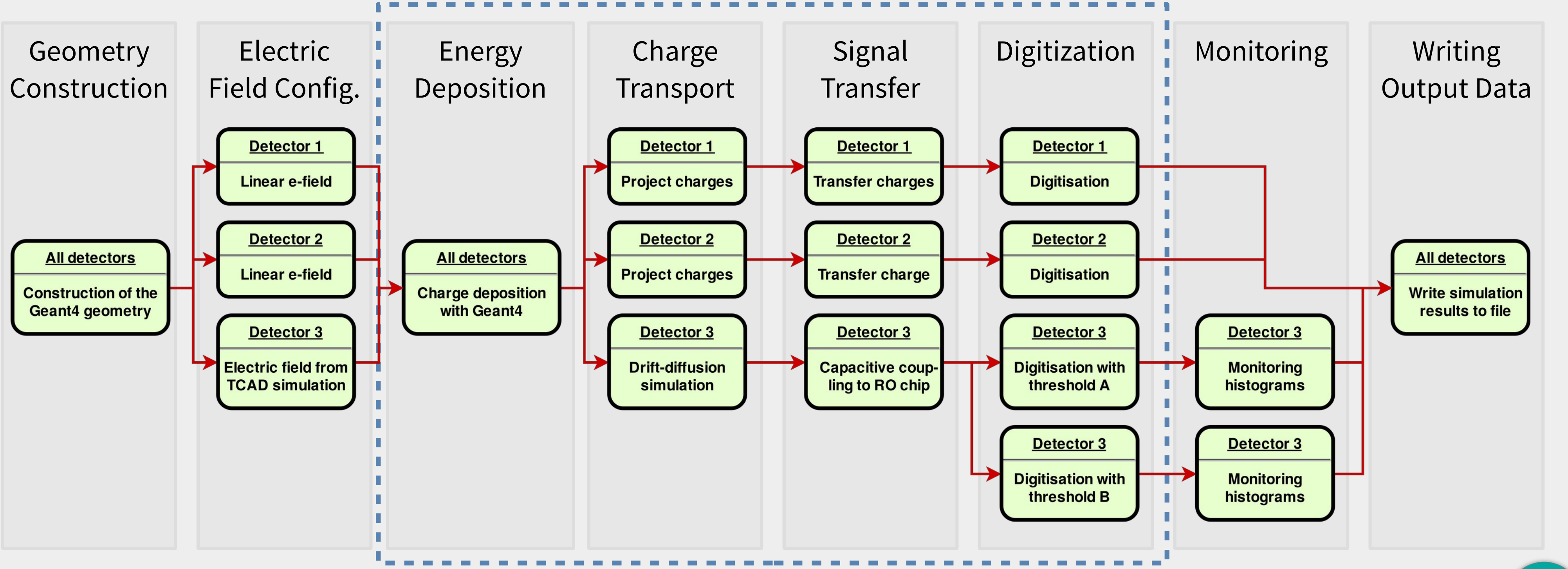
The Simulation Chain

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



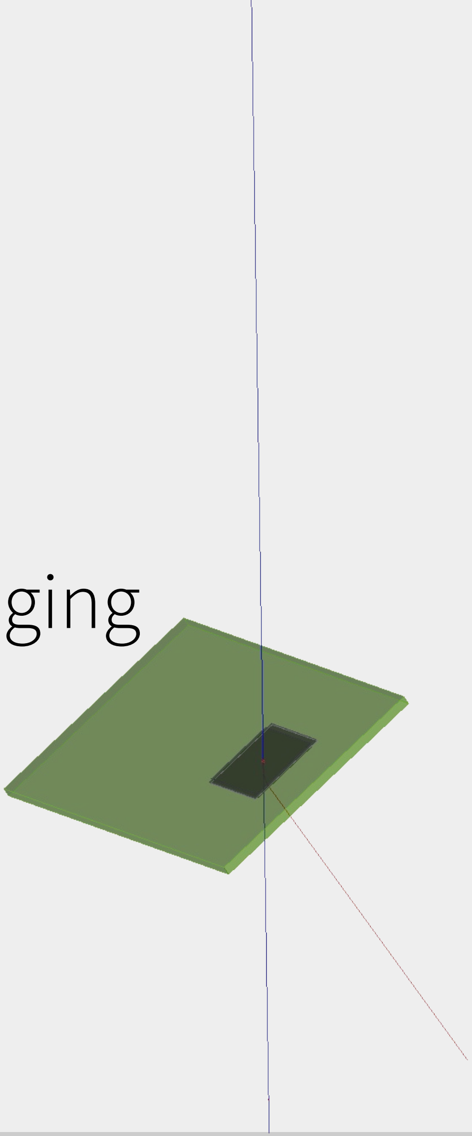
The Simulation Chain

- Simulation very flexible: modules configurable on per-detector level
- Multiple instances can be run in at the same time (e.g. to simulate different front-ends)



Application Examples

MAPS Sensors, PET Scanners, Neutron Imaging

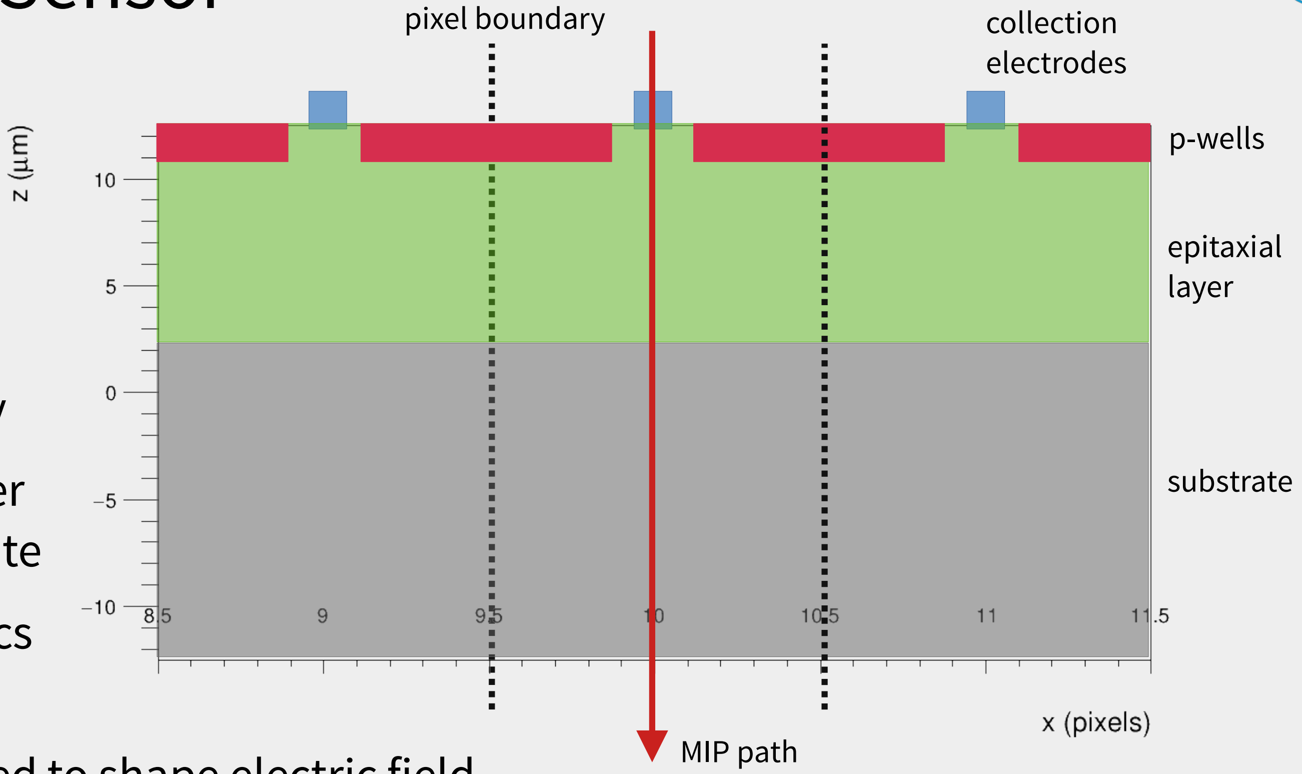


Simulating a MAPS Sensor

MAPS sensors are complex…

Example:

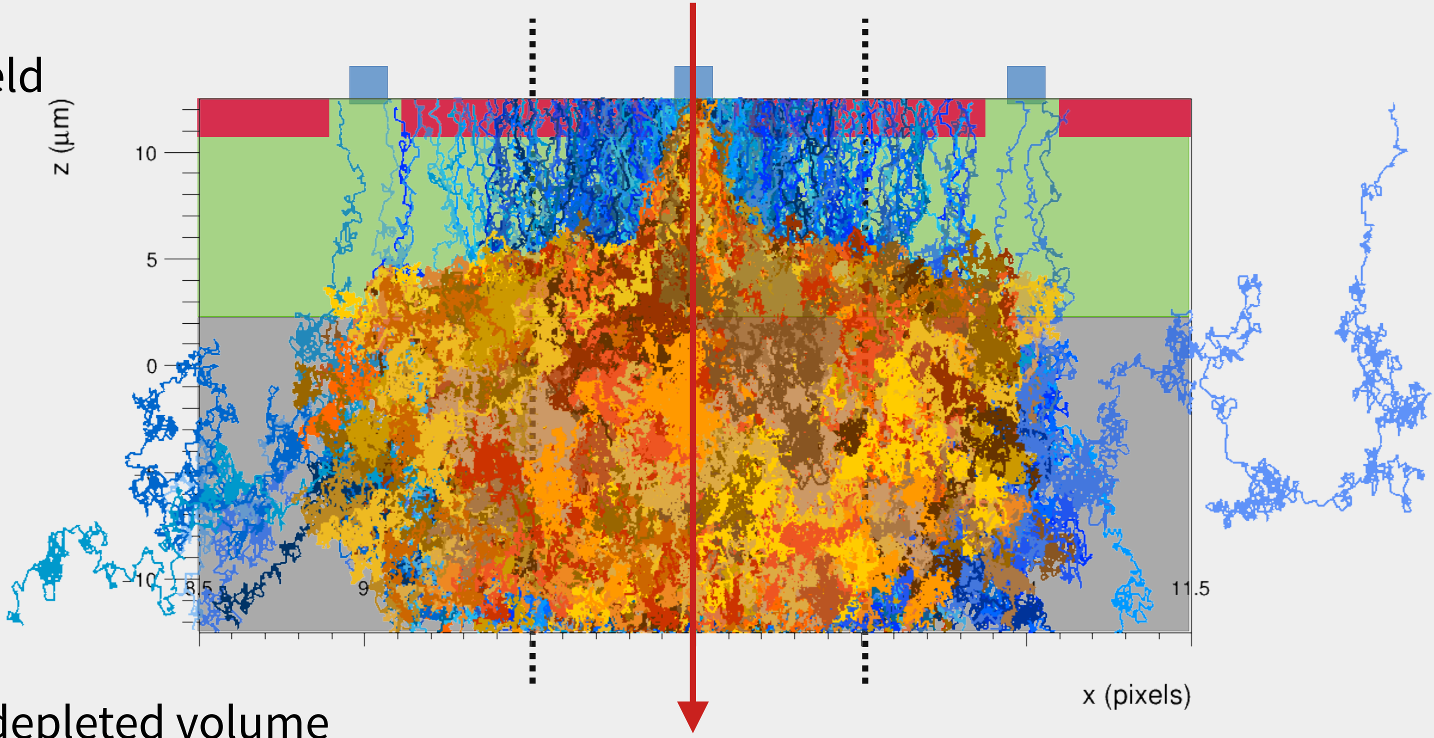
- Small-electrode sensor in CMOS Imaging technology
- High-resistivity epitaxial layer on electronics-grade substrate
- Deep wells protect electronics circuit from sensor field
- Additional implantations used to shape electric field



Simulating response to minimum ionizing particle incident perpendicular to surface

Simulating a MAPS Sensor – Simplistic Approach

- Applying linear electric field
    - Bias voltage -1.2 V
    - Depletion depth 10 µm
- Carrier mobility:
    - Canali model
    - Integrating for 50 ns

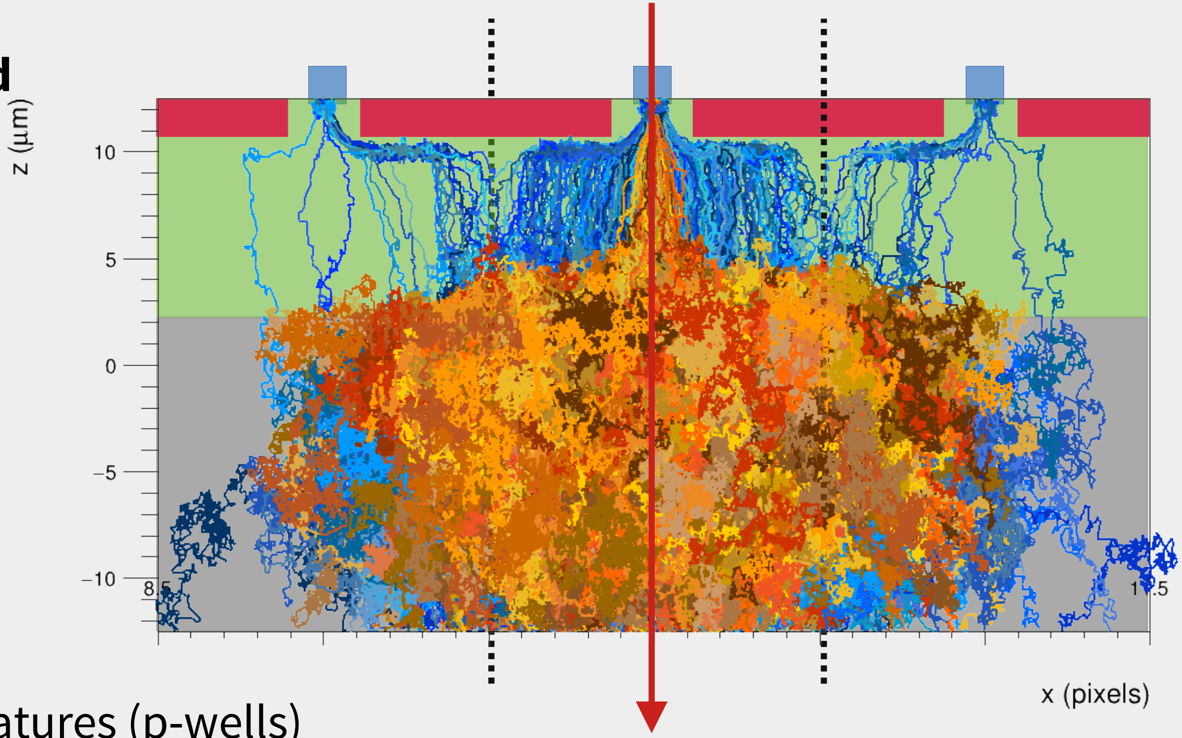


🟦 electrons
🟧 holes

- Diffusion dominant in undepleted volume
- Linear drift of charge carriers towards sensor surface, no drift to electrodes
- Large charge cloud, significant signal contribution from substrate

Simulating a MAPS Sensor – The Electric Field

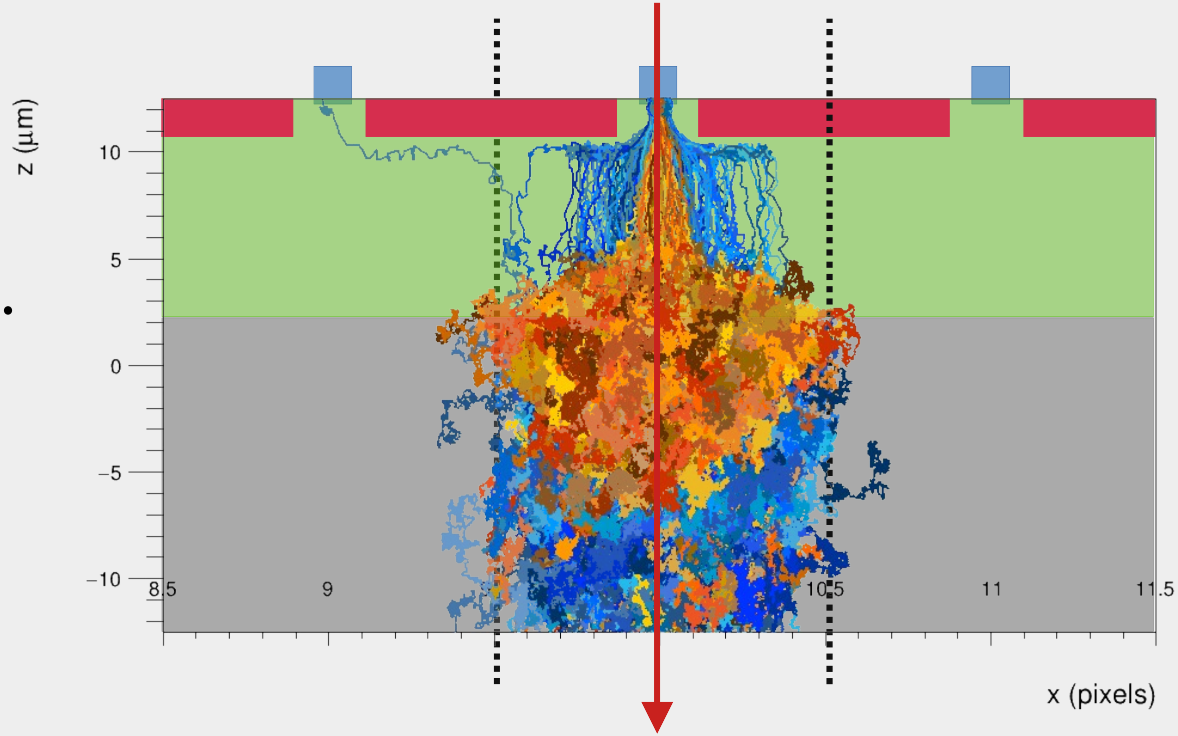
- Applying **TCAD electric field**
  - Bias voltage -1.2 V
  - Depletion depth 10 µm
- Carrier mobility:
  - Canali model
  - Integrating for 50 ns



- Carrier drift obeys sensor features (p-wells)
- Collection at electrodes
- Still signal contribution from substrate

Simulating a MAPS Sensor – Epi & Substrate Doping

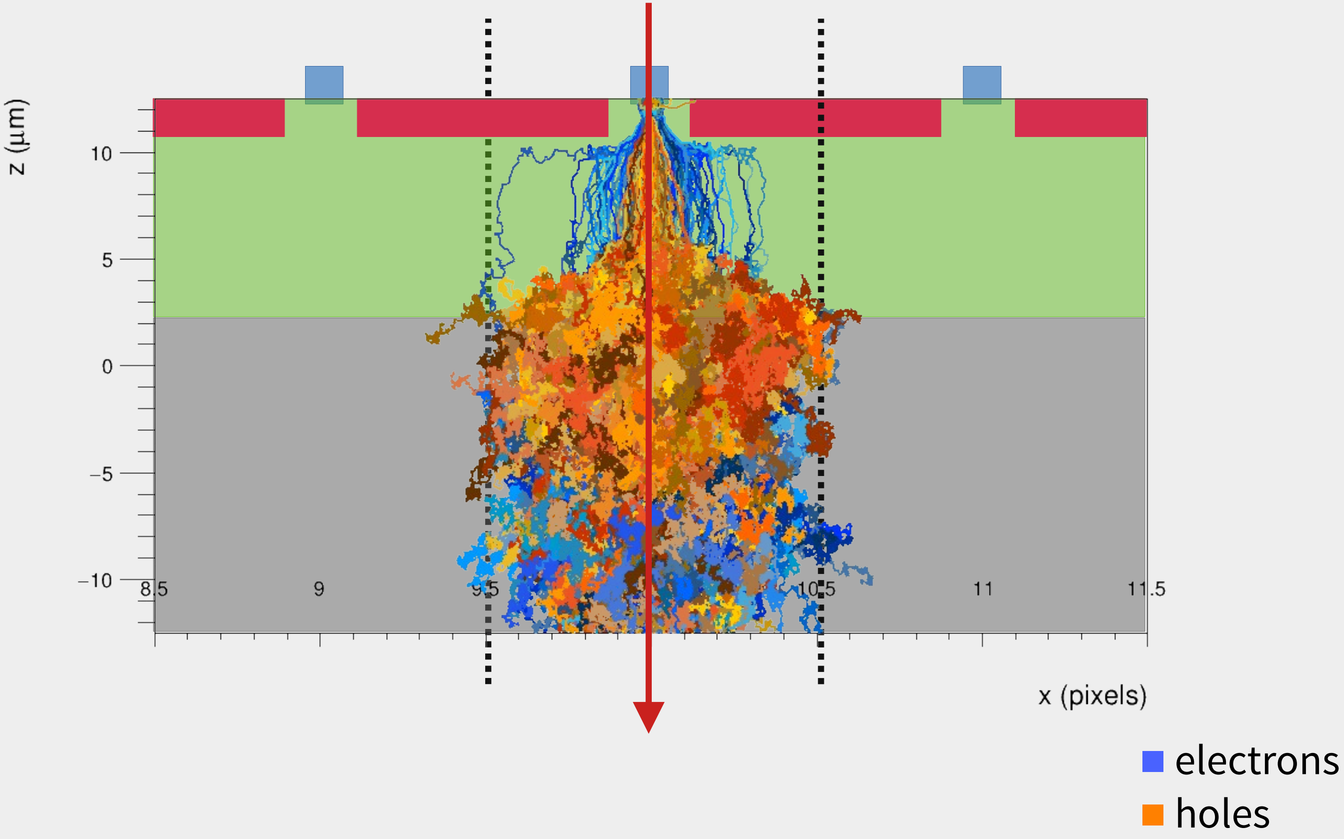
- Applying TCAD electric field
  - Bias voltage -1.2 V
  - Depletion depth 10 μm
- Setting **doping for epi & subs.**
- Carrier mobility:
  - **Masetti-Canali** model (doping dependent)
  - Integrating for 50 ns



- Significant reduction of diffusion in highly-doped substrate
- Less charge sharing from substrate contributions

Simulating a MAPS Sensor – Carrier Lifetime

- Applying TCAD electric field
  - Bias voltage -1.2 V
  - Depletion depth 10 µm
- Setting doping for epi & subs.
- Carrier mobility:
  - Masetti-Canali model (doping dependent)
  - Integrating for 50 ns
- **Recombination: combined SRH-Auger** model

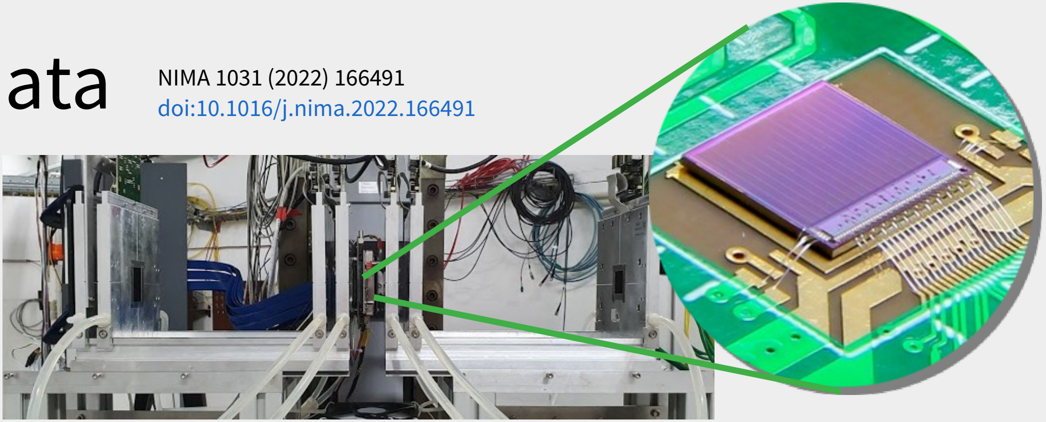


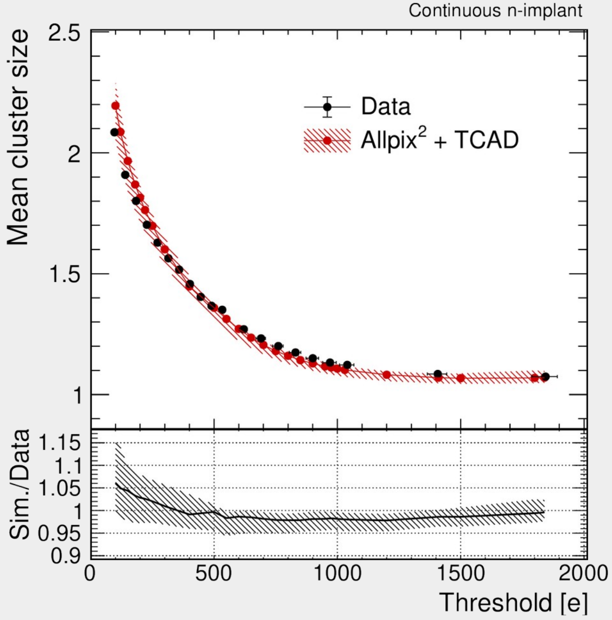
- Significant reduction of substrate contributions due to short lifetime in high-doping volume

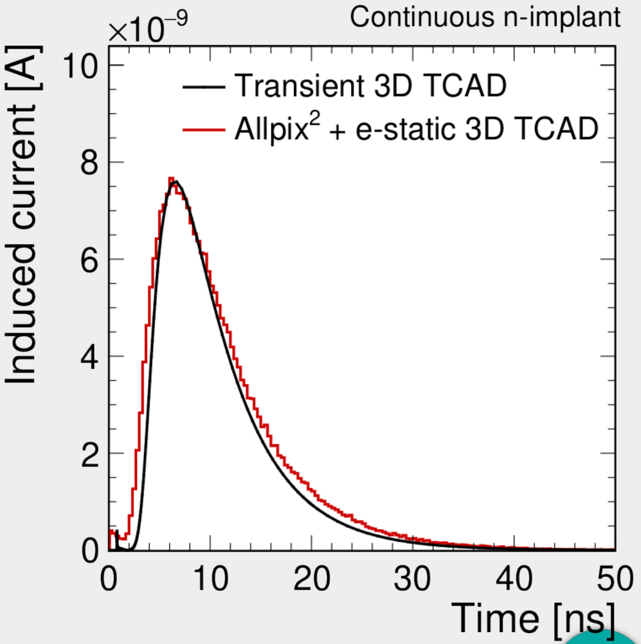
Comparison with Testbeam Data

NIMA 1031 (2022) 166491
doi:10.1016/j.nima.2022.166491

- CLICTD prototype for CLICdet tracking detector
- Validation of MC simulation with data recorded at DESY II Testbeam
    - Excellent match of position resolution as function of threshold
- Comparison of TCAD transient simulation with Shockley-Ramo MC simulation
    - Very good match, also across different sensor designs





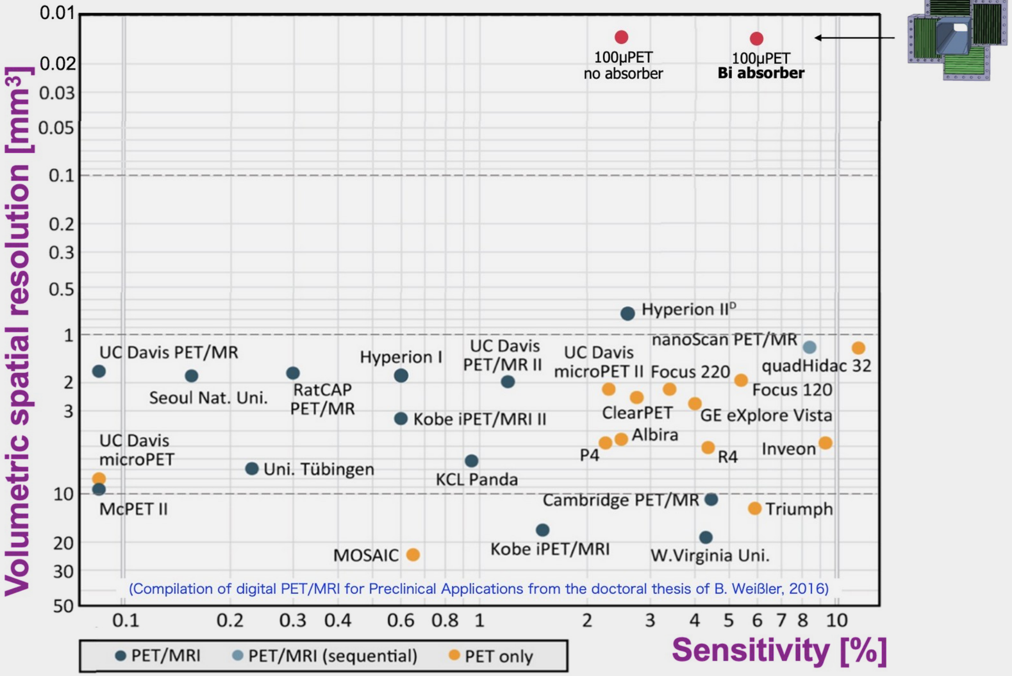


The 100µPET Project

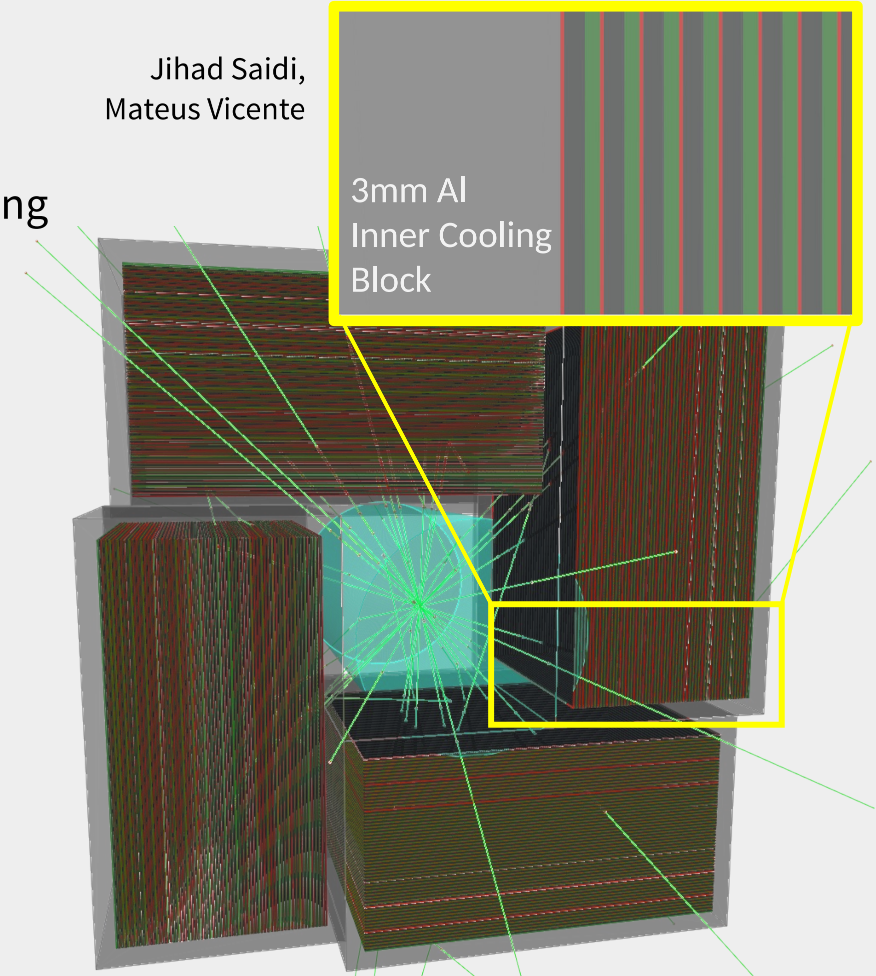
Jihad Saidi,
Mateus Vicente

New generation of PET scanners for high-res. molecular imaging

- 4 Sectors, each 60 detection layers, monolithic Si sensors
- Layer of 250 µm active silicon, 20 µm SiO2, 200 µm Kapton, 50 µm Bi



(Compilation of digital PET/MRI for Preclinical Applications from the doctoral thesis of B. Weißler, 2016)

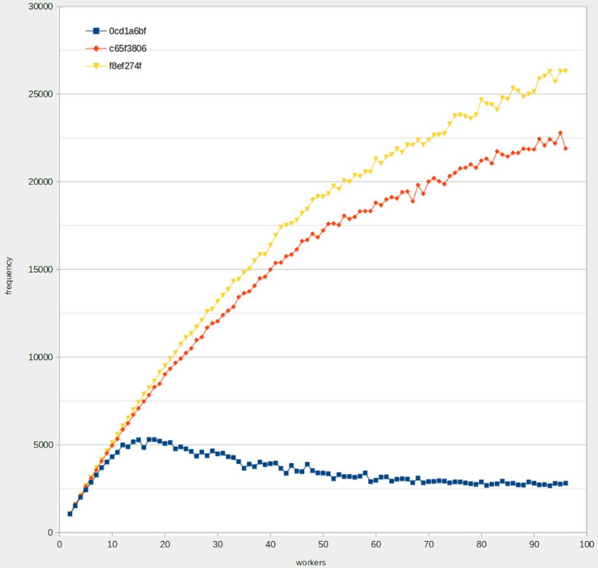


UNIVERSITÉ DE GENÈVE

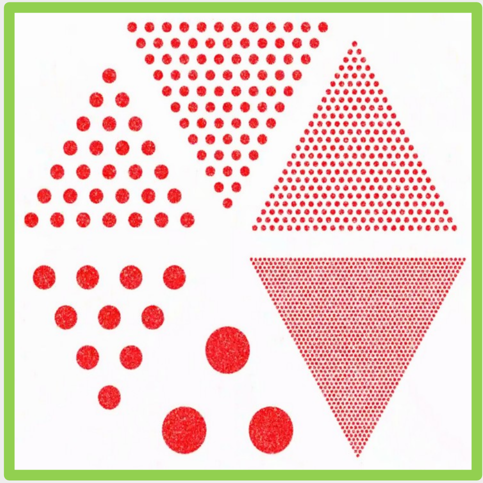
Simulating the 100µPET Scanner

Jihad Saidi,
Mateus Vicente

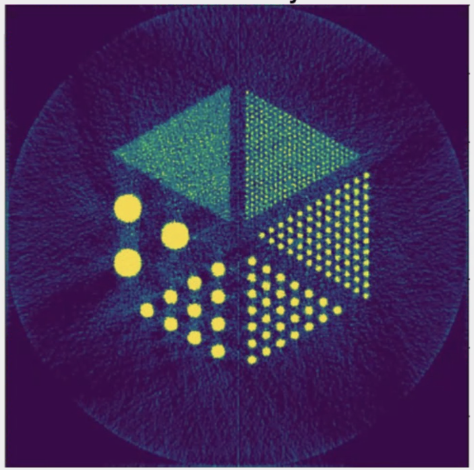
- Simulating full setup with Allpix Squared
  - Script to generate geometry setup
    Placement of sensors, support, absorbers
  - Interaction from Geant4 module:
    Positron annihilation and MFP, Photon Interactions
  - Charge carrier propagation
  - Electronics response
    (pixel threshold 10 keV)
  - Clustering
- Custom particle sources:
  images to simulate realistic phantoms
- High-rate event generation for
  "realistic data-sets" with ~10^9 events



De Renzo Phantom



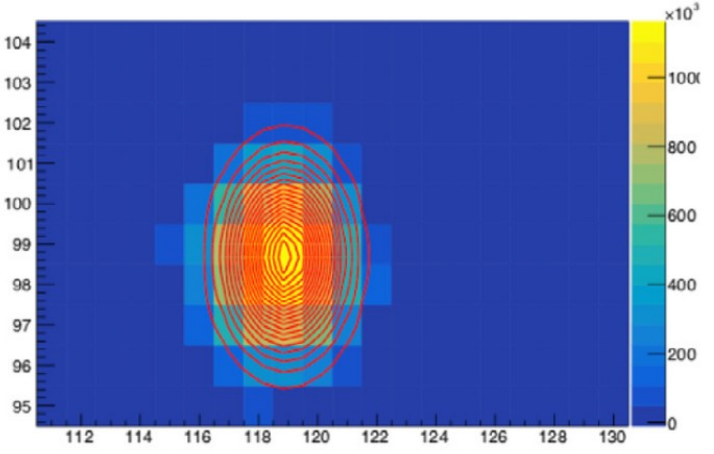
Iterative + sensitivity-corrected



Machine Learning for Neutron Position Resolution

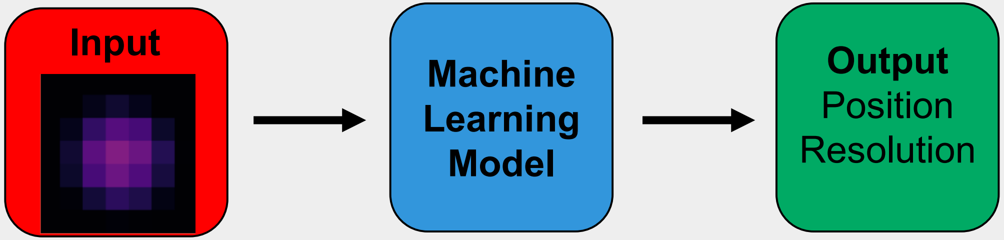
Shanny Lin,
Zhehui Wang

- High spatial resolution of ultracold neutron (UCN) measurements is crucial for several experiments involving UCNs such as quantum physics and quantum gravity
- Previous work uses a 2D Gaussian fit to determine hit position
- **Goal:** use machine learning and Allpix Squared to predict hit position while accounting for detector physics



2D gaussian fitted to a UCN hit

NIMA 1003 (2021) 165306
doi:10.1016/j.nima.2021.165306



Input

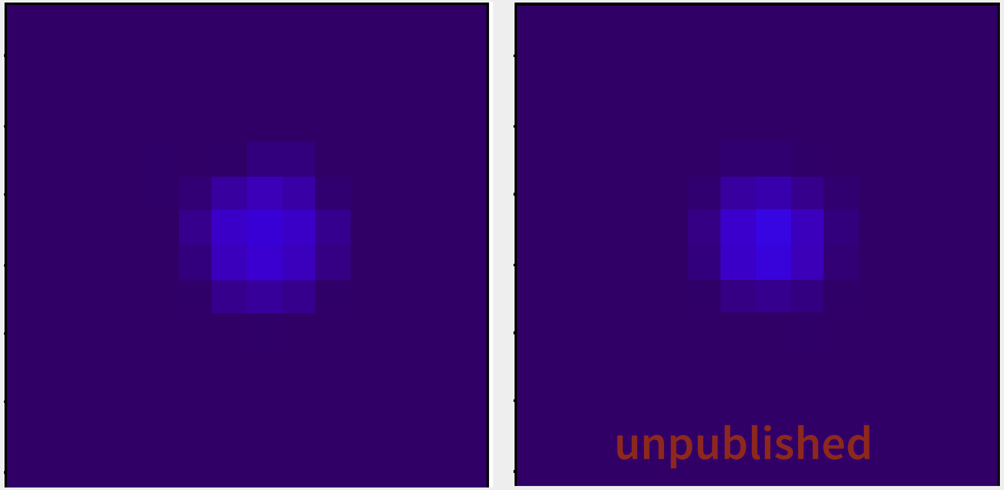
Machine Learning Model

Output Position Resolution

Allpix Squared for Neutron Imaging: Highlights

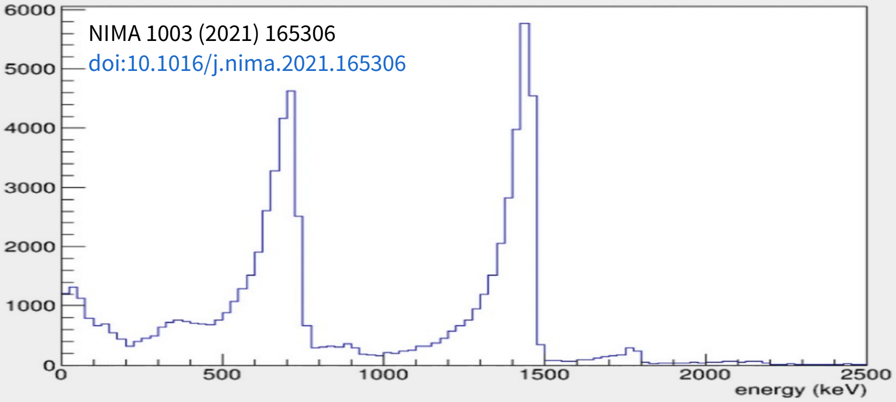
Shanny Lin,
Zhehui Wang

UCN Hit Images:



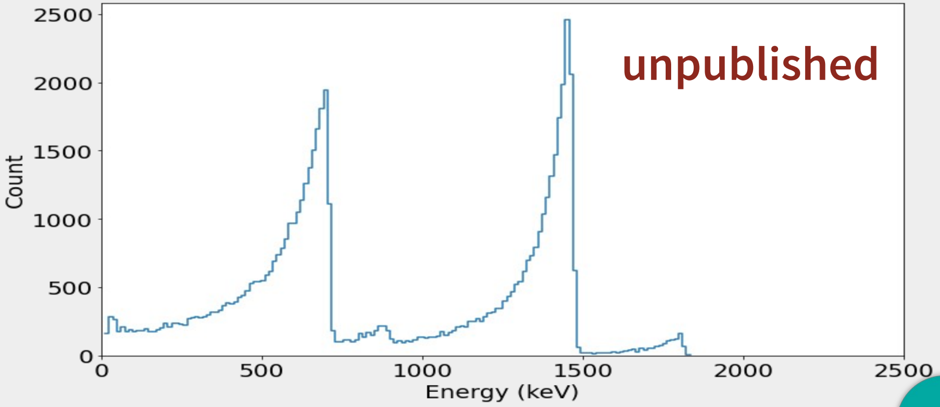
Experimental vs Allpix Squared

Experimental Energy Spectrum



NIMA 1003 (2021) 165306
doi:10.1016/j.nima.2021.165306

Simulated Energy Spectrum



Ongoing Developments

and Recent Features

```
odule {
end class ModuleManager;
end class Messenger;


ief Base constructor for unique modules
am config Configuration for this module

t Module(Configuration& config);

 Base constructor for detector modules
 config Configuration for this module
 detector Detector bound to this module
g Detector modules should not forget to forward their detector to the base c
 \ref InvalidModuleStateException will be raised if the module failed to so

dule(Configuration& config, std::shared_ptr<Detector> detector);

sential virtual destructor.

es all delegates linked to this module

e();



 a module is not allowed

le&) = delete;
(const Module&) = delete;




ve behaviour (not possible with references)

cept = delete;
le&&) noexcept = delete;
```

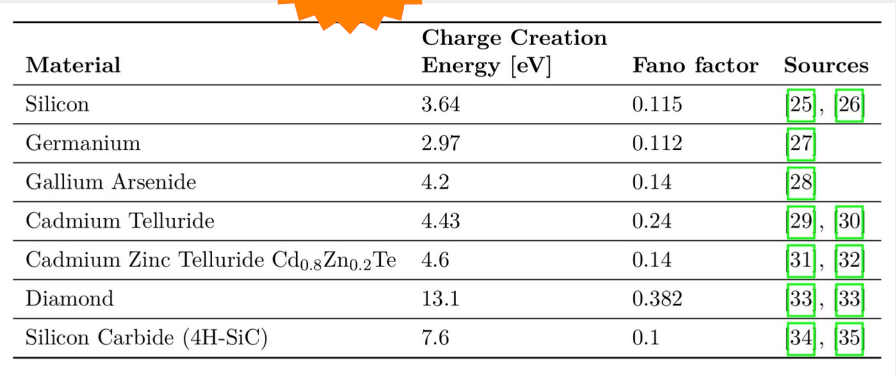
Other Semiconductor Sensor Materials

v2.3

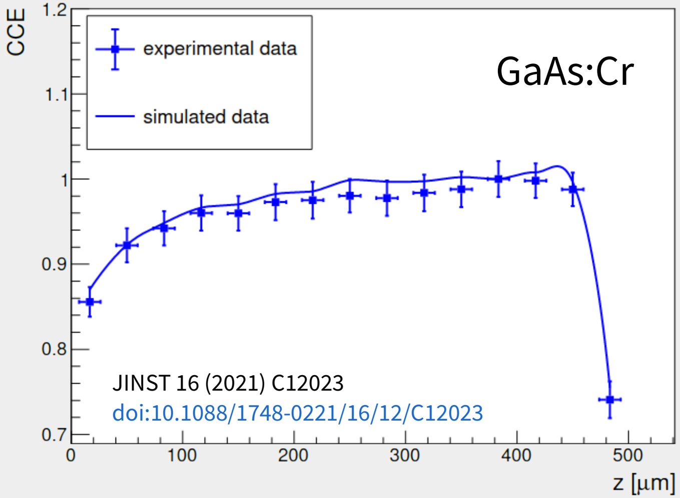
Paul Schütze,
Petr Smolyanskiy

Allpix^2 ~~Silicon~~ Semiconductor Detector Simulation Framework

- Selection of sensor material in det. model
- Definition of sensor materials impacts …
  - Material in Geant4 geometry
  - Charge carrier creation energy default
  - Fano factor default
  - Mobility model, recombination, …
- Benchmark simulation using GaAs:Cr sensors show very good agreement



Material	Charge Creation Energy [eV]	Fano factor	Sources
Silicon	3.64	0.115	[25], [26]
Germanium	2.97	0.112	[27]
Gallium Arsenide	4.2	0.14	[28]
Cadmium Telluride	4.43	0.24	[29], [30]
Cadmium Zinc Telluride $Cd_{0.8}Zn_{0.2}Te$	4.6	0.14	[31], [32]
Diamond	13.1	0.382	[33], [33]
Silicon Carbide (4H-SiC)	7.6	0.1	[34], [35]



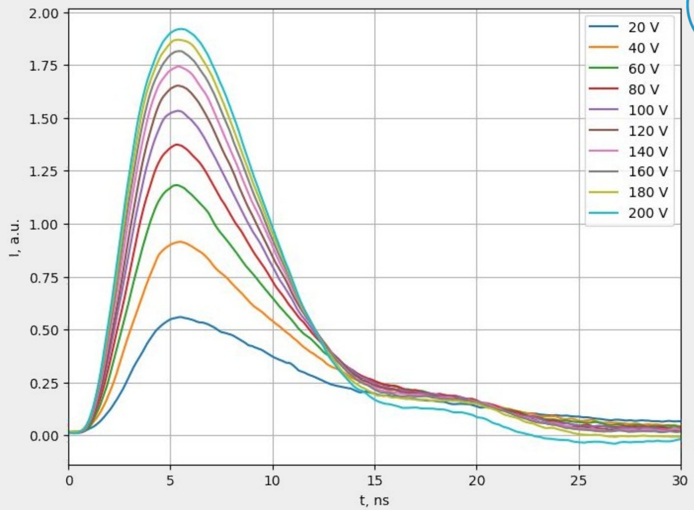
GaAs:Cr

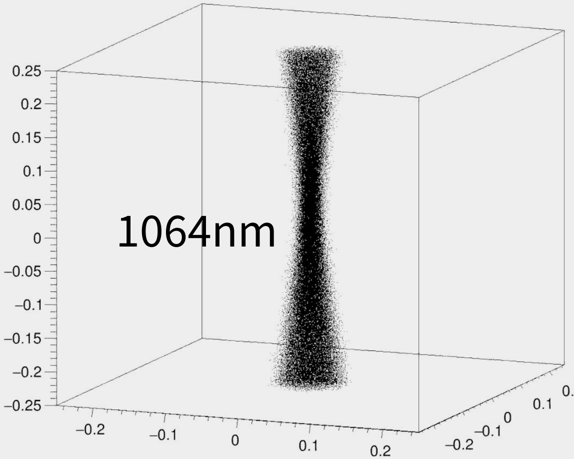
JINST 16 (2021) C12023
doi:10.1088/1748-0221/16/12/C12023

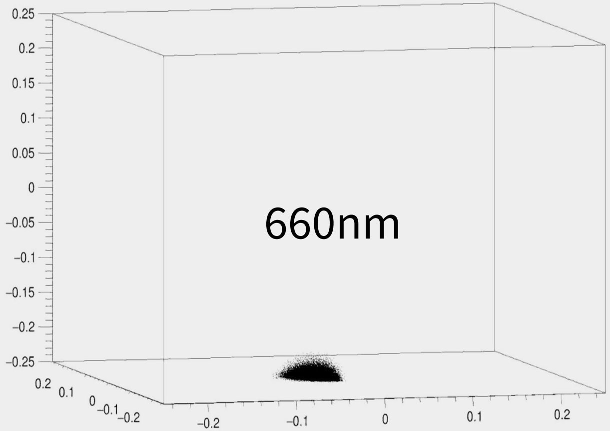
Daniil Rastorguev

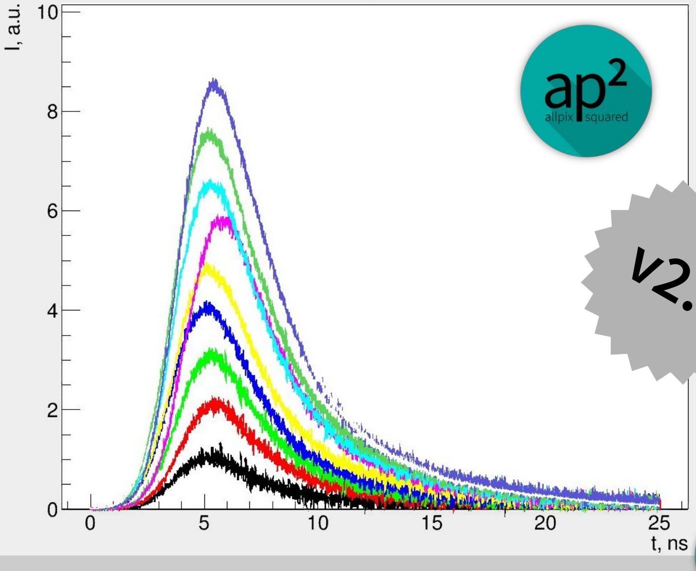
Simulation of TCT & Lasers

- Simulate interaction of visible/near-IR light with sensors
- Implemented as separate deposition module
- Pulse with individual photons generated over time
- Penetration depth, refraction simulated, different beam geometries & wavelengths possible:









v2.4

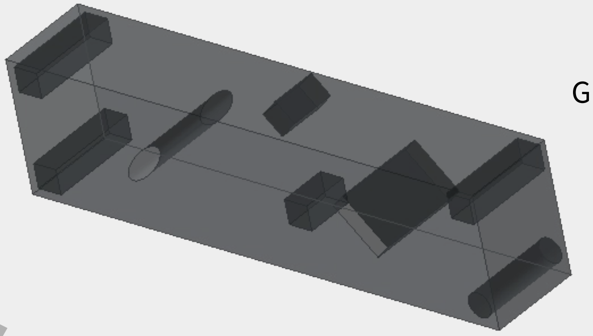
Simulation of 3D Sensors

Marco Bomben,
Gilberto Giuliarelli,
Gian-Franco Dalla Betta

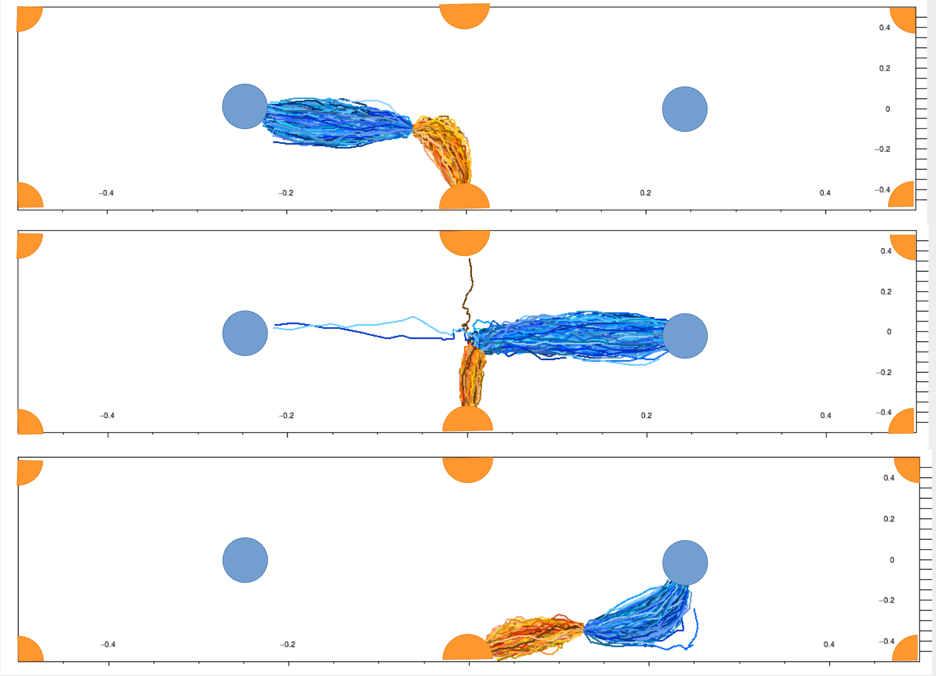
- Definition of per-pixel implants via detector model
  - Position with respect to pixel center
  - Shape & orientation
  - Material
  - front/backside
- Add as many implants as required, syntax similar to support layers (PCB etc)
- Collision detection of charge carriers with implants; motion stops immediately at implant border

v3.0

- First simulations with ATLAS 3D sensor geometry
  - Two central front-side columns (collect charge)
  - Six Ohmic backside contact columns



single pixel,
top projection of 3D drift



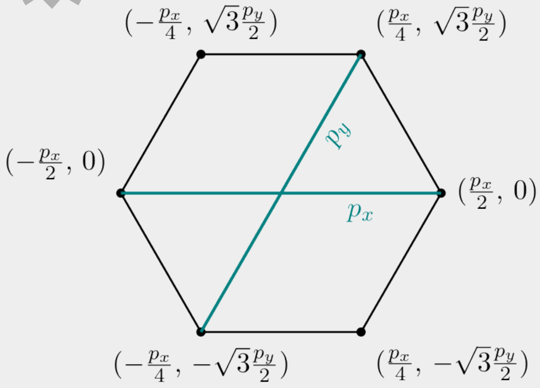
Hexagonal Pixel Geometries

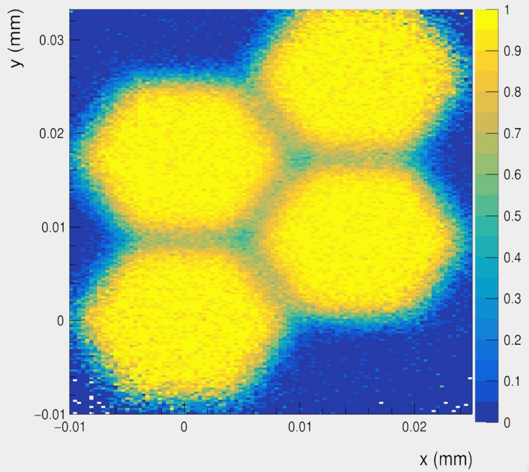
v3.0

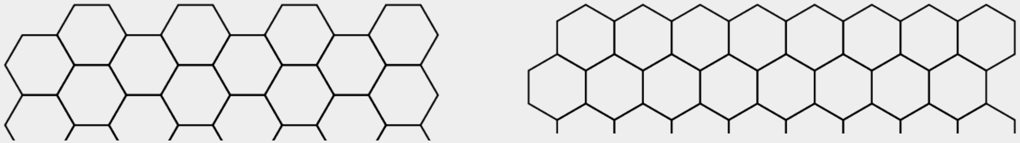
Katharina Dort,
Paco Iguaz-Gutierrez,
Ryuji Moriya,
Tasneem Saleem

Extension of geometry subsystem to enable simulation of different pixel shapes & matrix arrangements

- Hexagonal geometry interesting for many applications
  - Avoid problematic field regions in corners
    (issues with electric fields, charge sharing between 4 pixels, …)
  - Symmetry more close to circle – more uniform response
- Implementation using **axial coordinate system**
- Support for “pointy” & “flat” hexagon orientation,
  regular (same-pitch) and distorted (different pitch) hexagons







Other geometries also implemented (e.g. radial strips @ ATLAS ITk)

Summary

Summary

- Semiconductor Detector Monte Carlo simulations:
  vital component of understanding & interpreting detector performance

- Allpix Squared:
  comprehensive MC simulation framework for semiconductor detectors
  - integrates existing toolkits
  - provides validated algorithms
  - is easy-to-get-started and well documented

- Used in many areas within & outside of particle physics
- Continuous development and support, many new features already underway

Use, spread, contribute!

This project has received funding from the European Union’s Horizon 2020
Research and Innovation programme under Grant Agreement No 101004761.

Allpix Squared Resources

Website

https://cern.ch/allpix-squared

Repository

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

Docker Images

https://gitlab.cern.ch/allpix-squared/allpix-squared/container_registry

User Forum:

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

Mailing Lists:

allpix-squared-users https://e-groups.cern.ch/e-groups/Egroup.do?egroupId=10262858

allpix-squared-developers https://e-groups.cern.ch/e-groups/Egroup.do?egroupId=10273730

User Manual:

https://cern.ch/allpix-squared/usermanual/allpix-manual.pdf


DESY.