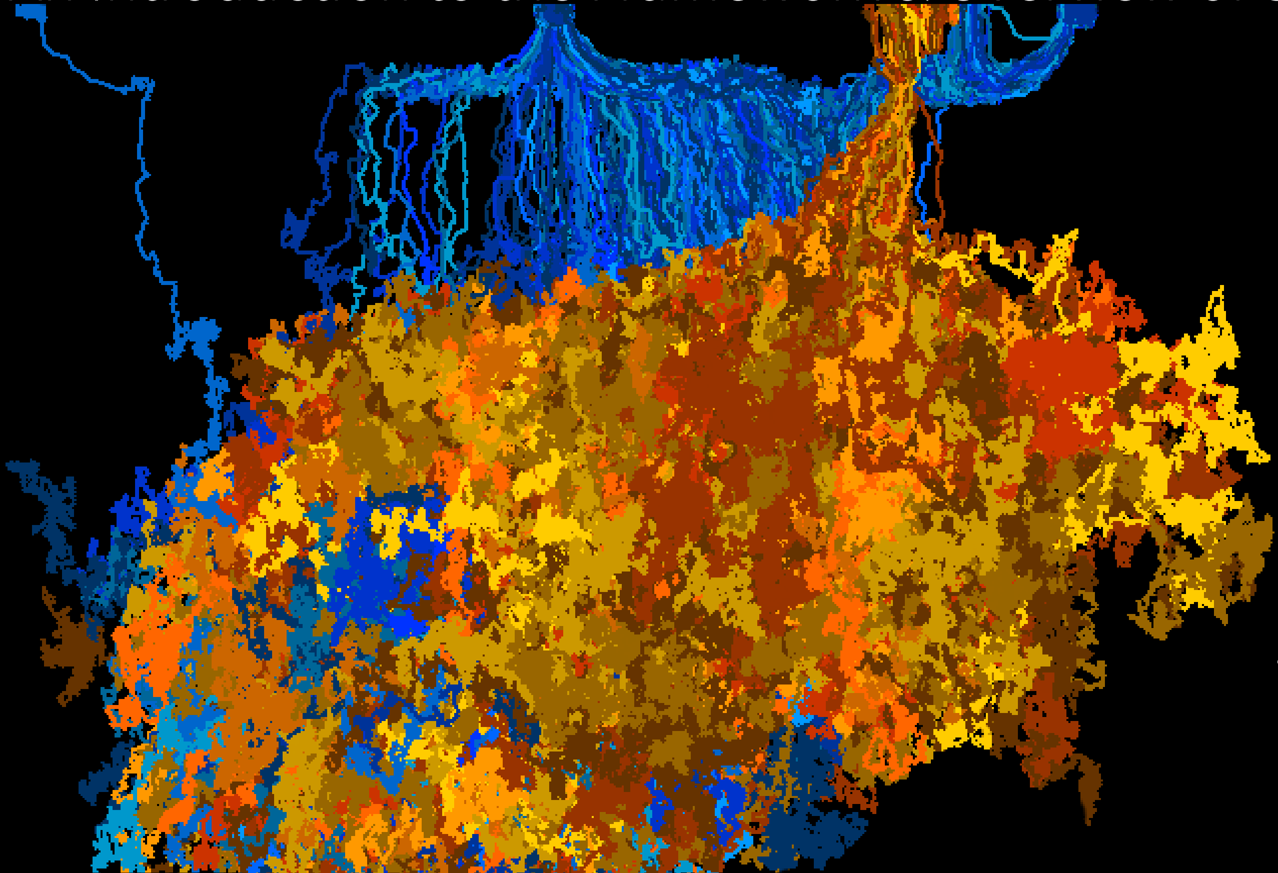
https://www.desy.de/

Allpix Squared 2.x

An Introduction to the Framework & Overview of Series-2.x Features



Simon Spannagel, DESY
for the Allpix Squared Authors

4th Allpix Squared User Workshop
DESY, Hamburg
22 May 2023

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
Maoqiang Jing, IHEP Beijing
Moritz Kiehn, Université de Genève

Rafaella Eleni Kotitsa, Université de Genève
Stephan Lachnit, DESY
Salman Maqbool, CERN Summer Student
Stefano Mersi, CERN
Ryuji Moriya, CERN Summer Student
Sebastien Murphy, ETHZ
Andreas Matthias Nürnberg, DESY
Sebastian Pape, TU Dortmund University
Marko Petric, CERN
Florian Michael Pitters, HEPHY
Radek Privara, Palacky University Olomouc
Nashad Rahman, The Ohio State University
Sabita Rao, GSDocs2020 Student
Daniil Rastorguev, DESY
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Andre Sailer, CERN

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Arka Santra, Weizman Institute
Enrico Jr. Schioppa, Unisalento and INFN Lecce
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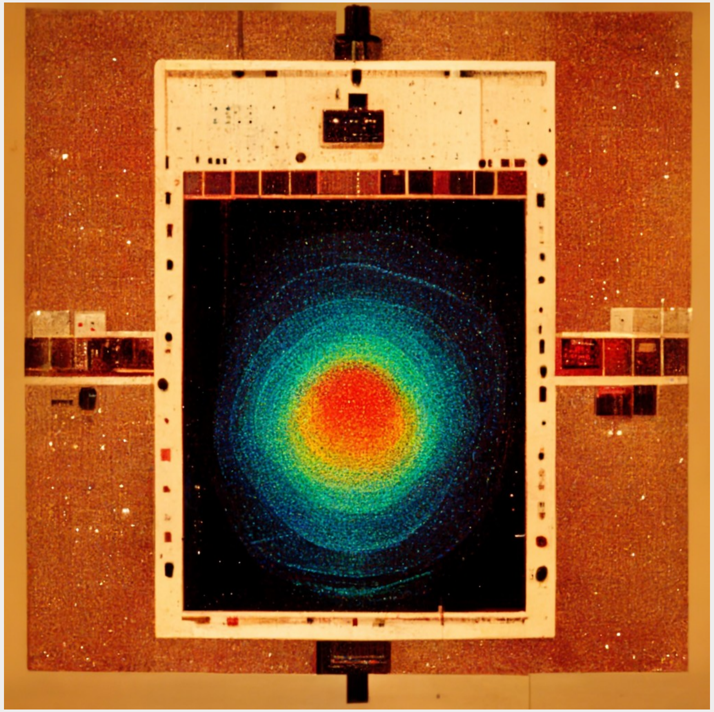
Mateus Vicente Barreto Pinto, Université de Genève
Håkan Wennlöf, DESY
Andy Wharton, Lancaster University
Morag Williams, University of Glasgow
Koen Wolters

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…



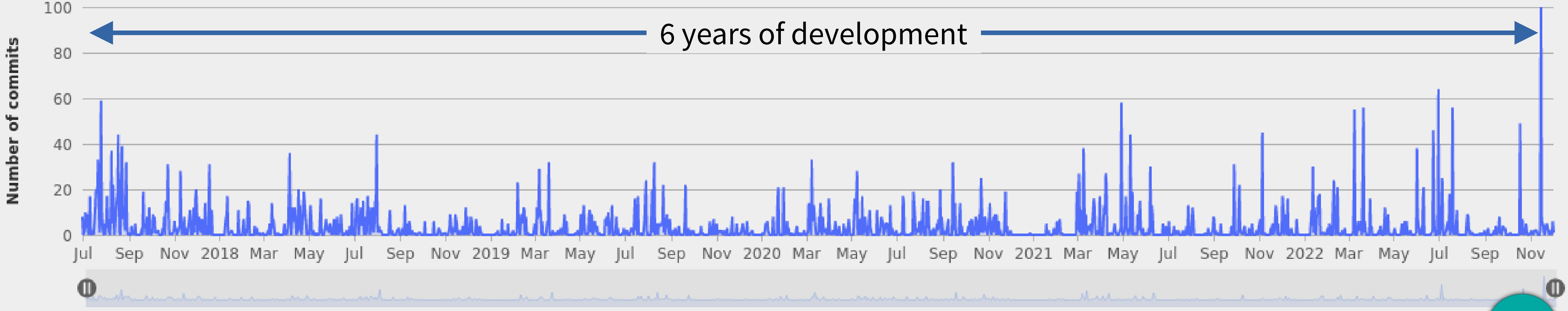
Midjourney,
`/image a silicon pixel detector measuring high-energetic particles`

The Allpix² Framework

- Development of entirely new framework
- Now 6 years of development with
  - 46 releases, current version 3.0.0
  - 4 user workshops
  - > 50 code contributors

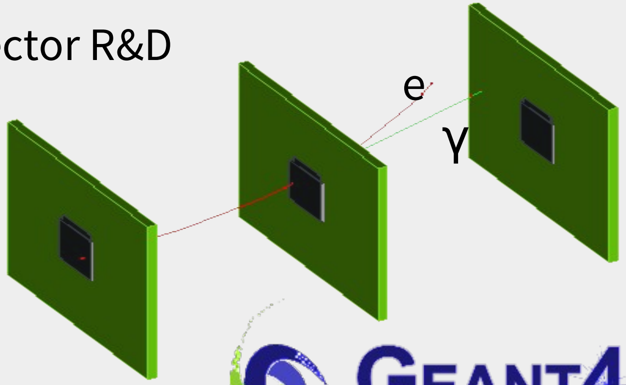
Development based on four principles:

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



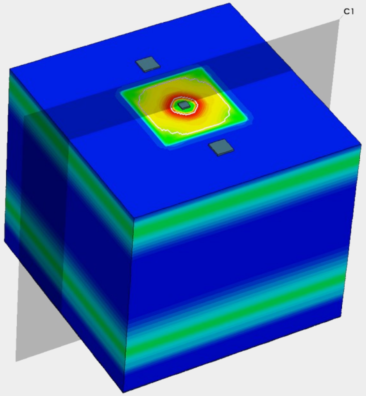
I. Integration of Existing Toolkits

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

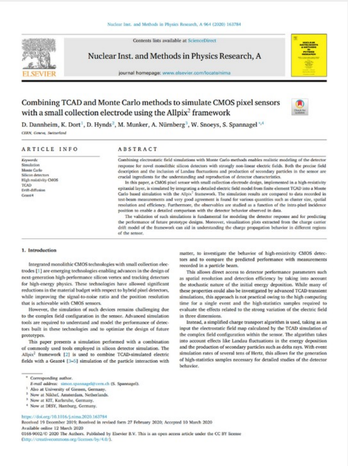
Simulations provide insights into physical processes – but only if they model them correctly!

- 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


Nuclear Inst. and Methods in Physics Research, A
Allpix²: A modular simulation framework for silicon detectors

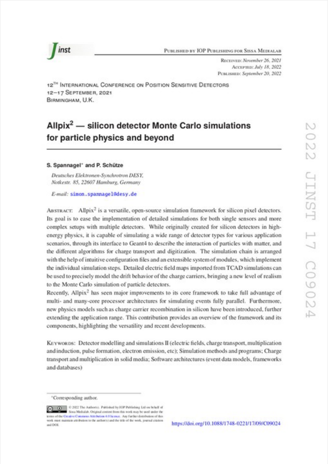
NIMA 901 (2018) 164 – 172
doi:10.1016/j.nima.2018.06.020


Nuclear Inst. and Methods in Physics Research, A
Combining TCAD and Monte Carlo methods to simulate CMOS pixel sensors with a small collection electrode using the Allpix² framework

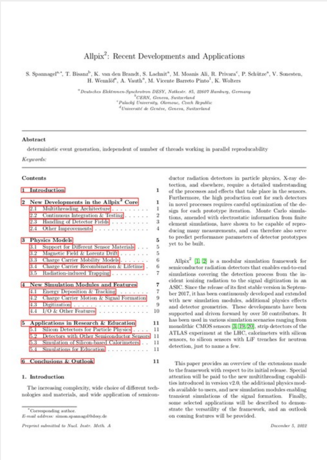
NIMA 964 (2020) 163784
doi:10.1016/j.nima.2020.163784


Nuclear Inst. and Methods in Physics Research, A
Transient Monte Carlo simulations for the optimisation and characterisation of monolithic silicon sensors

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


Allpix² — silicon detector Monte Carlo simulations for particle physics and beyond
S. Spannagel and P. Schütze

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


Allpix²: Recent Developments and Applications

In preparation…

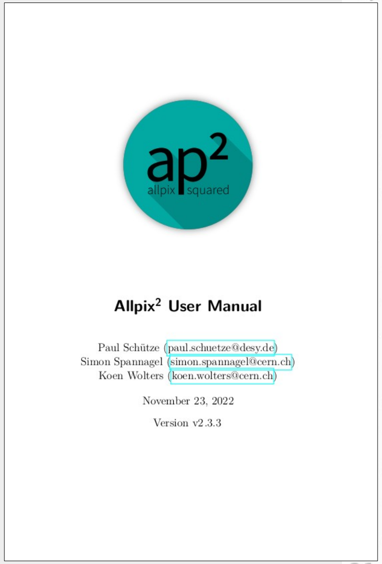
III. Low Entry Barrier for New Users

Simulation frameworks often very complex:

- complex code base, lack of documentation
- many physical effects to be simulated

- 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

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



Allpix^2 User Manual

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Koen Wolters (koen.wolters@cern.ch)

November 23, 2022

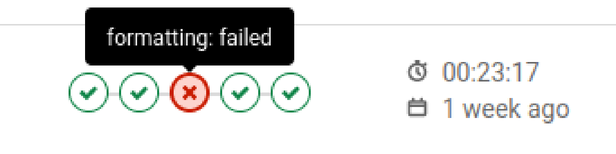
Version v2.3.3

```
[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]
```

Bonn-Cologne Graduate School of Physics and Astronomy

IV. Clean & Maintainable Code

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



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

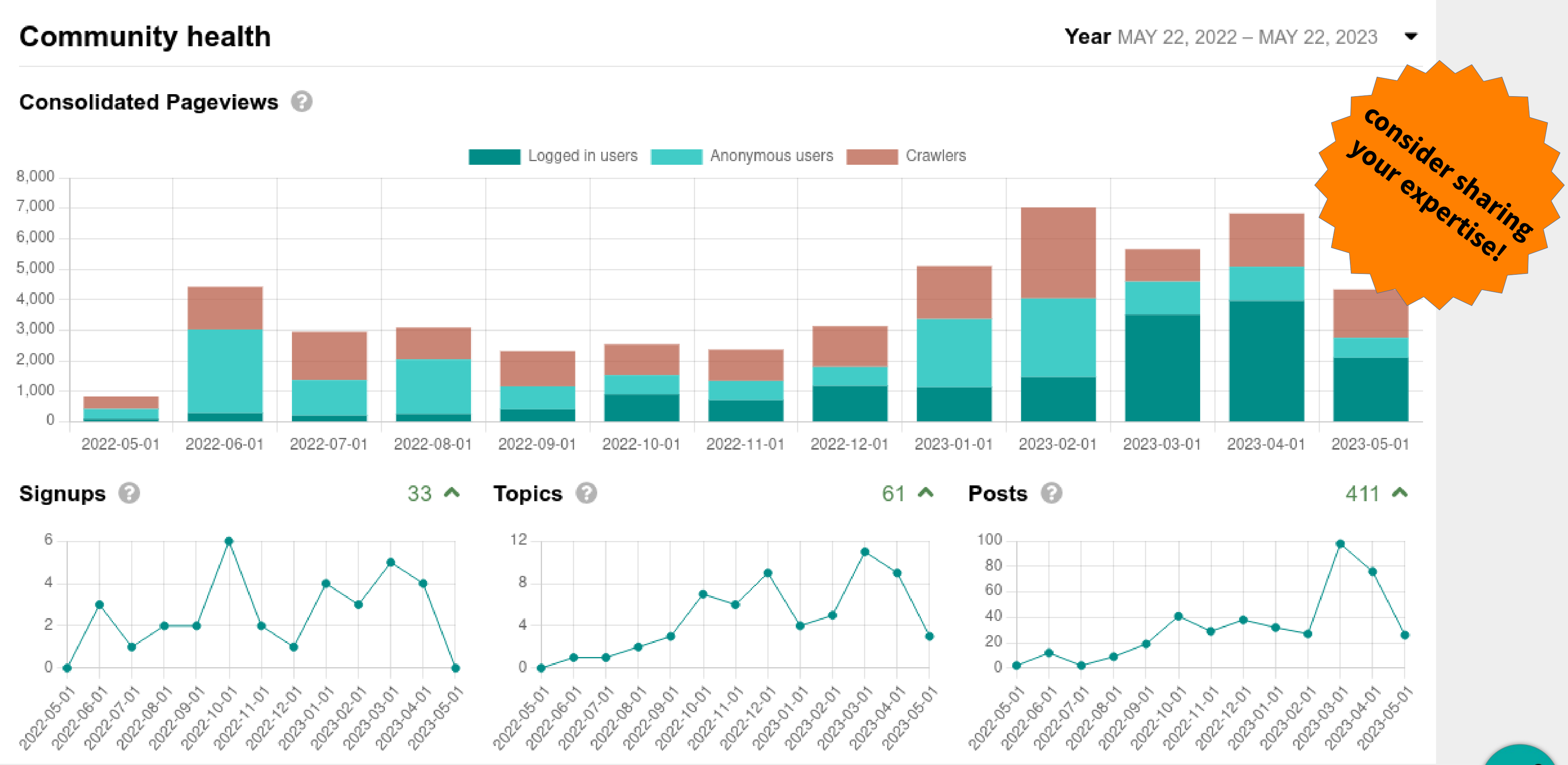
[v2.4-stable] Adding output plots to [DopingProfileReader]
!908 · created 2 weeks ago by Haakan Wennloef v2.4-stable backport improvement

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

“Community Health” – the APSQ Forum



Ongoing Developments
and Recent Features

Release of Allpix Squared 2.3

- Released on 16/05/2022, three subsequent patch releases
- Support for Semiconductor Sensor Materials
  - Silicon, Gallium Arsenide, Germanium, Cadmium Telluride, CdZnTe, Diamond, Silicon Carbide
  - Ionization energy, Fano factors as well as some mobility models provided
  - Dedicated section in user manual detailing materials, entry in FAQ describes procedure to use them as sensor
- SRH Recombination rate now scaling with temperature
- Implementation of “standard” low-fluence models for radiation-damage induced trapping, along with possibility to define custom formula

- Detailed release notes: https://cern.ch/allpix-squared/post/2022-05-16-allpix-squared-2.3-released/

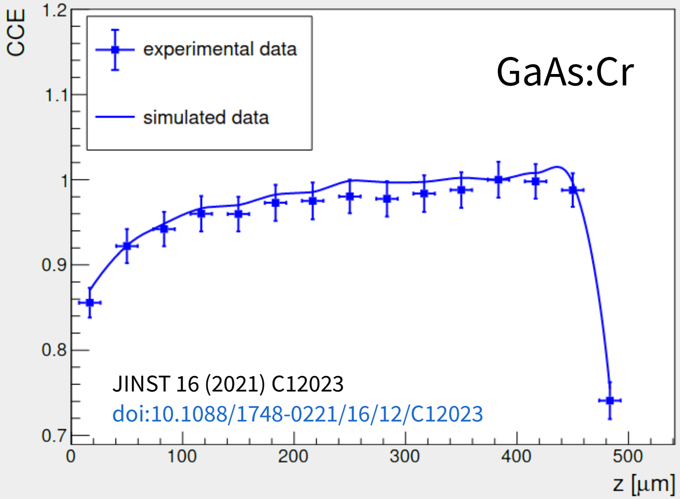
Other Semiconductor Sensor Materials

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]



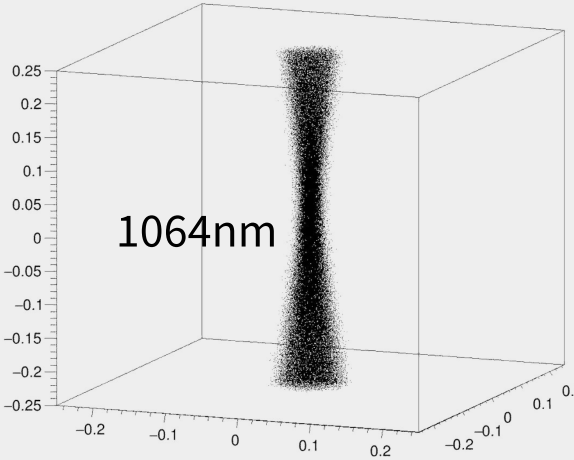
Release of Allpix Squared 2.4

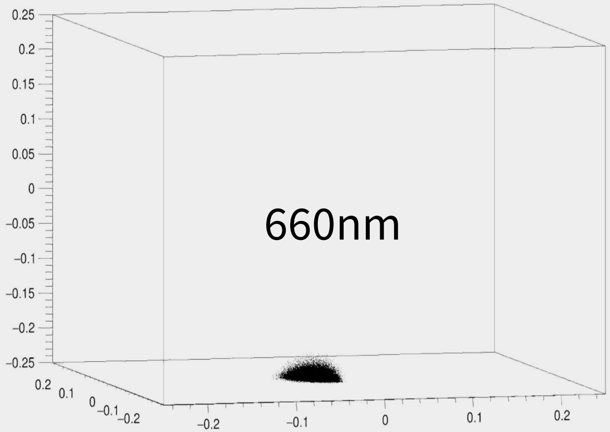
- Released on 12/01/2023
- New module: DepositionGenerator
  - Module to read primary particles from MC generators sch as Pythia
  - Using Geant4 to propagate through setup
  - Allows easier integration into existing simulation toolchains
- New module: DepositionLaser
  - Module to simulate laser & TCT measurements
  - Includes refraction, focusing, absorption, temporal pulse distribution

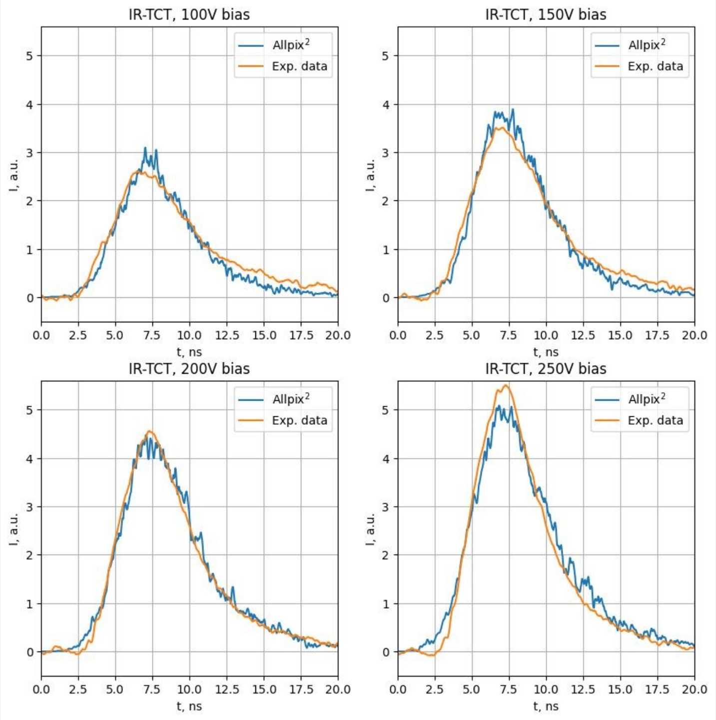
- Detailed release notes:
  https://cern.ch/allpix-squared/post/2023-01-12-allpix-squared-2.4-released/

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
- See talk by Daniil

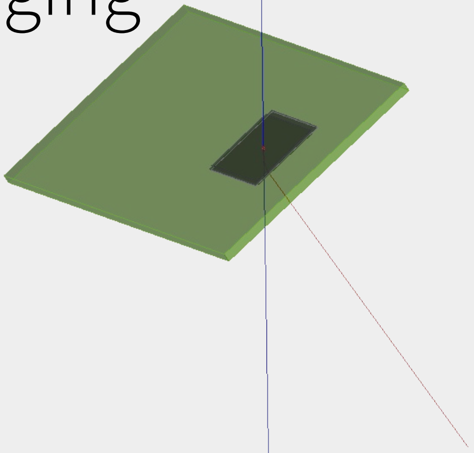






Application Examples

MAPS Sensors, PET Scanners, Neutron Imaging

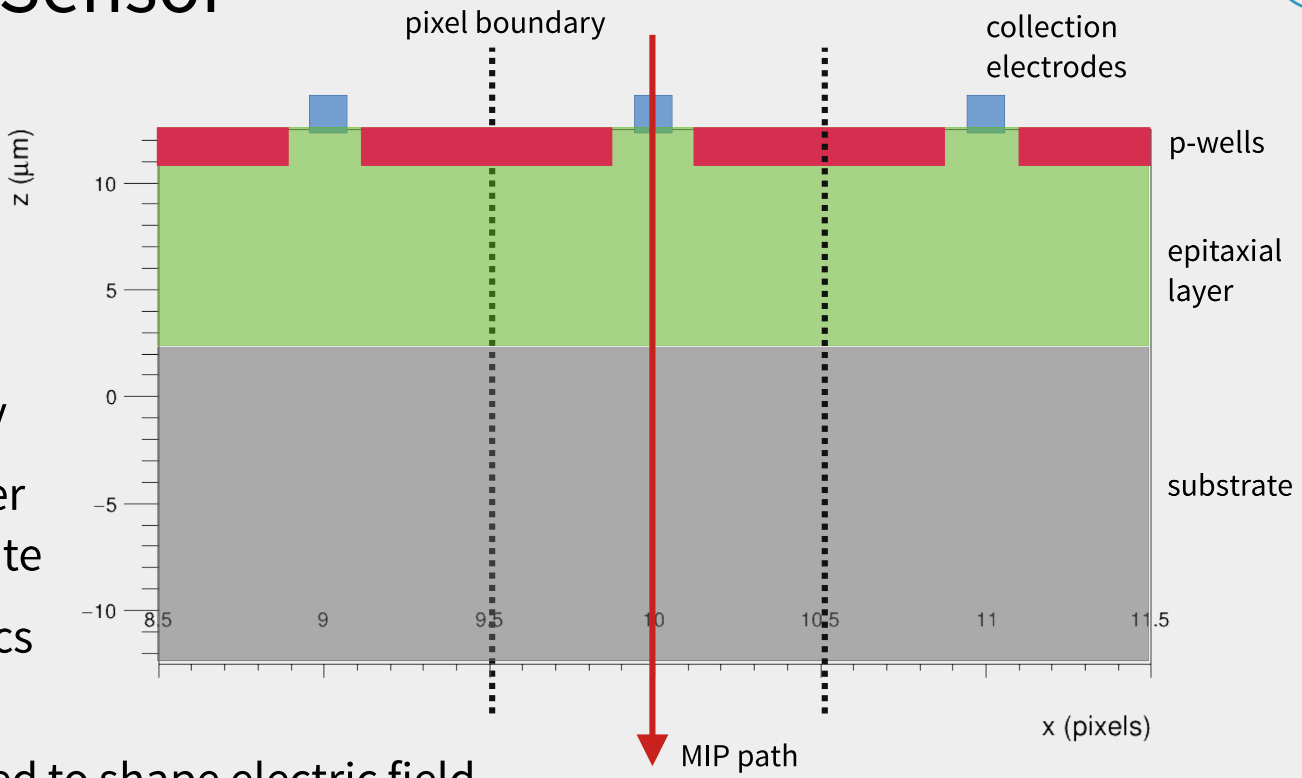


Simulating a MAPS Sensor

MAPS sensors are complex…

Example:

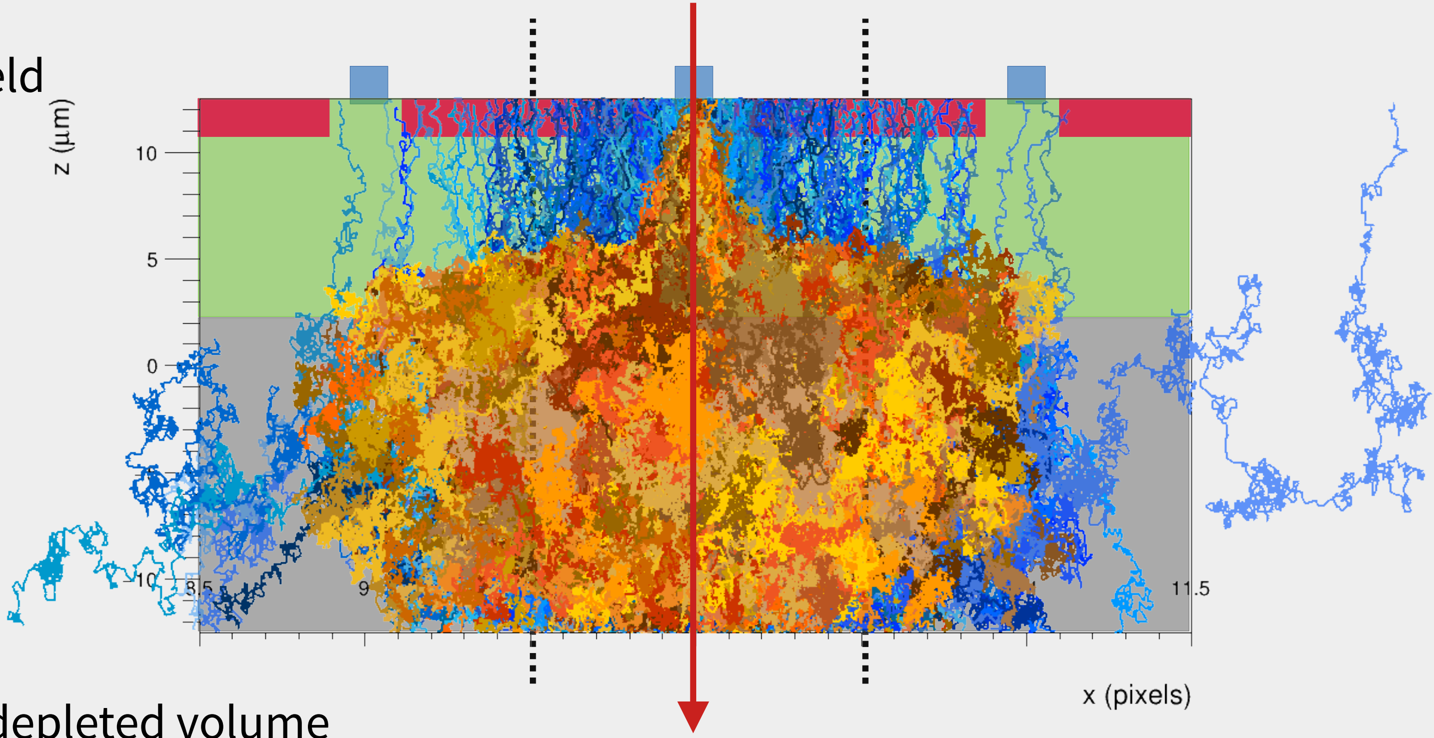
- Small-electrode sensor in CMOS Imaging technology
- High-resistivity epitaxial layer on electronics-grade substrate
- Deep wells protect electronics circuit from sensor field
- Additional implantations used to shape electric field



Simulating response to minimum ionizing particle incident perpendicular to surface

Simulating a MAPS Sensor – Simplistic Approach

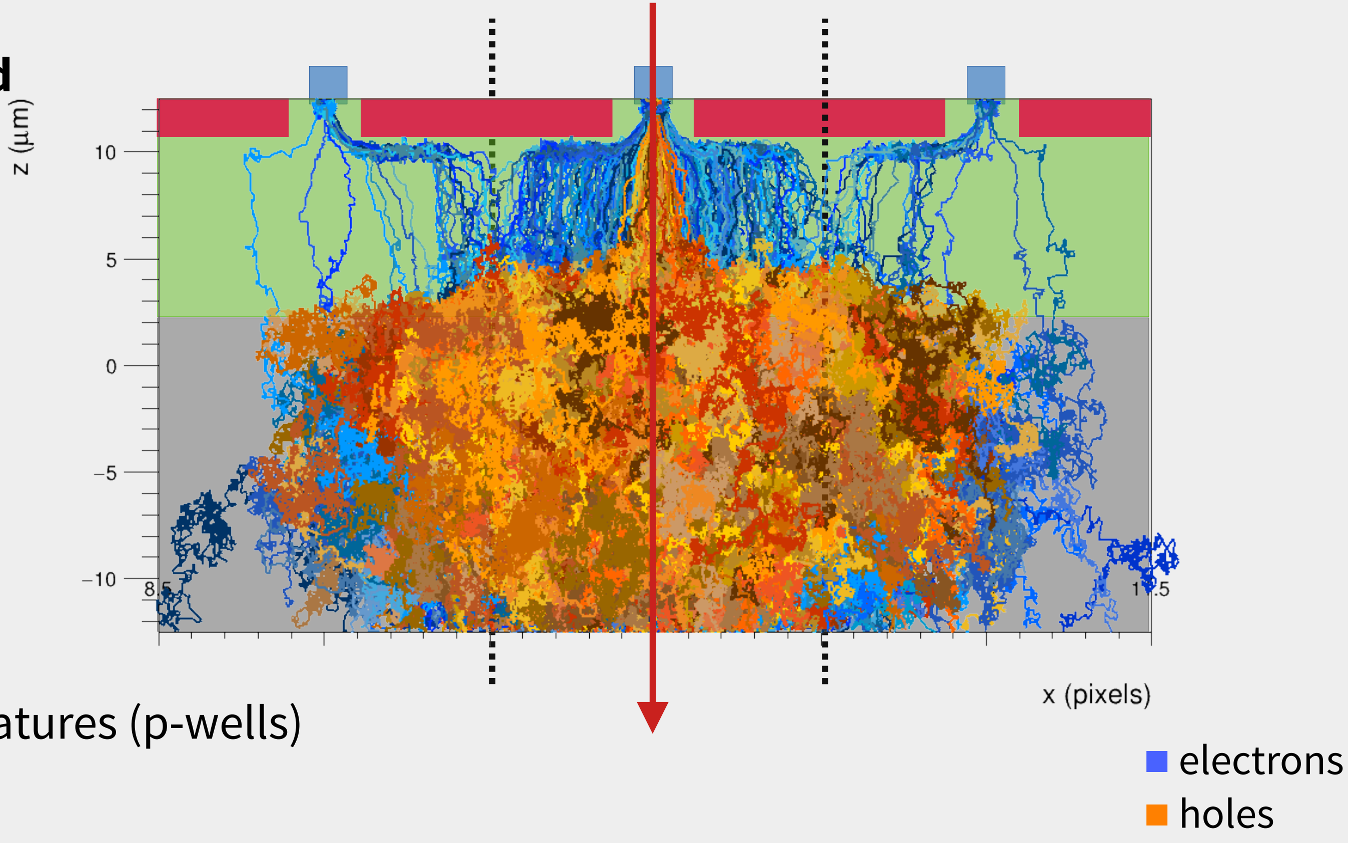
- Applying linear electric field
  - Bias voltage -1.2 V
  - Depletion depth 10 µm
- Carrier mobility:
  - Canali model
  - Integrating for 50 ns



- 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

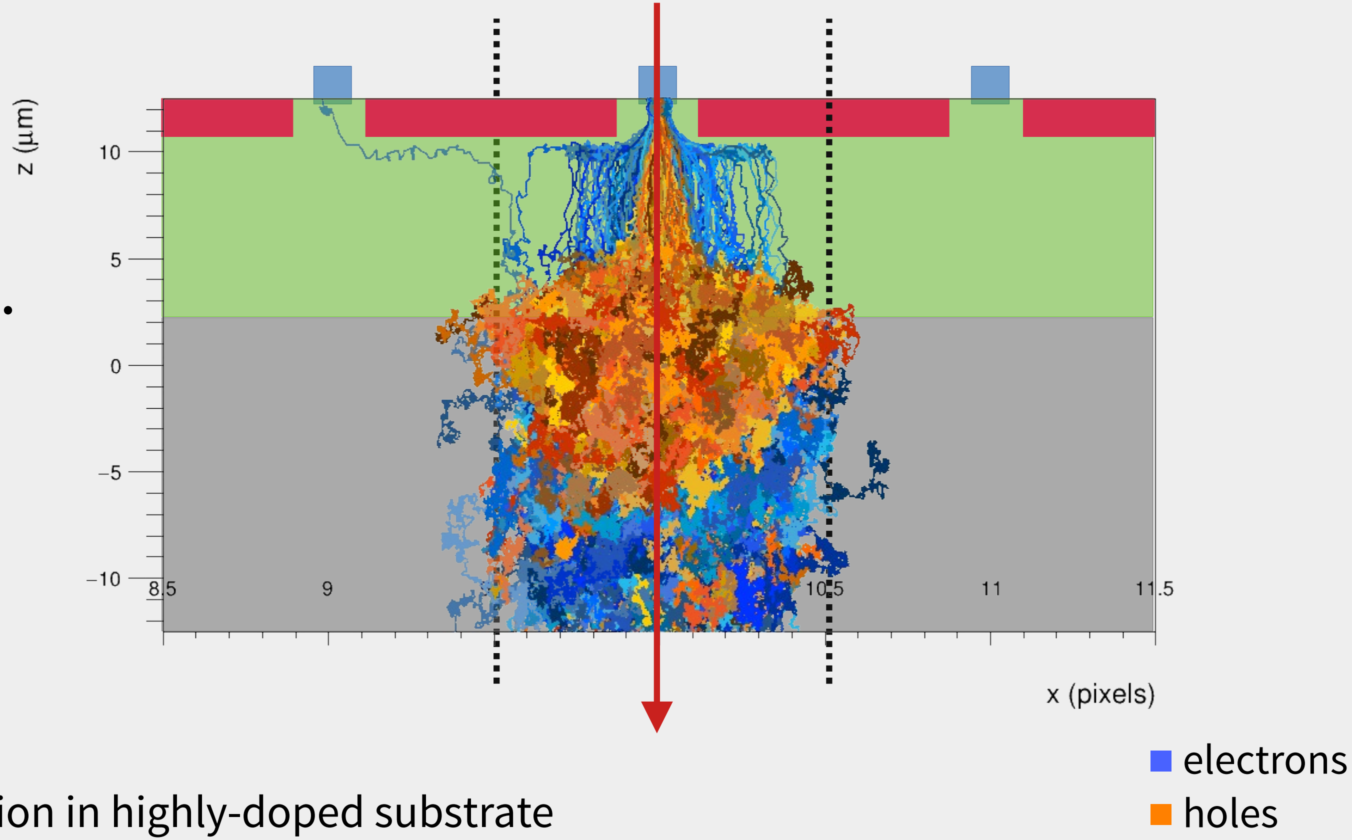
- Applying **TCAD electric field**
  - Bias voltage -1.2 V
  - Depletion depth 10 µm
- Carrier mobility:
  - Canali model
  - Integrating for 50 ns



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

Simulating a MAPS Sensor – Epi & Substrate Doping

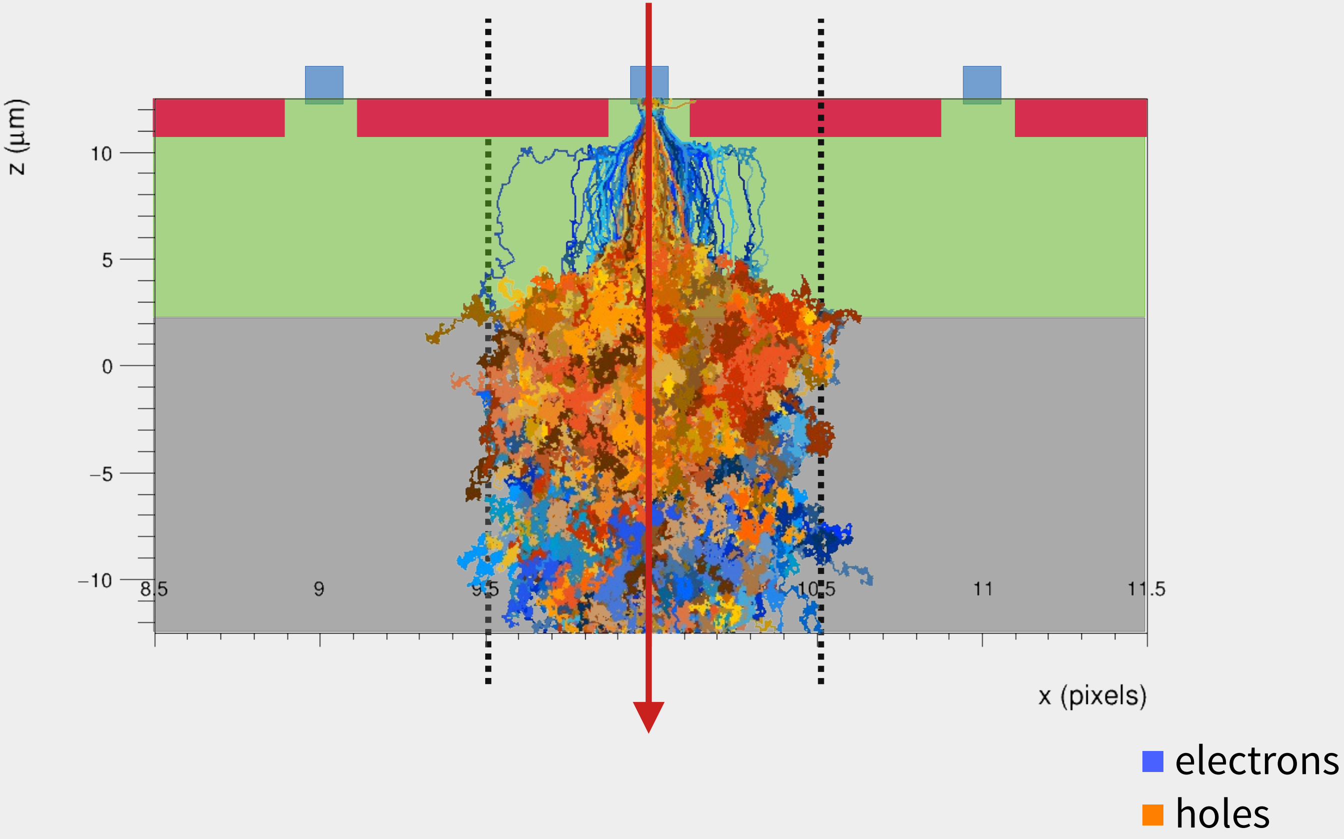
- Applying TCAD electric field
  - Bias voltage -1.2 V
  - Depletion depth 10 μm
- Setting **doping for epi & subs.**
- Carrier mobility:
  - **Masetti-Canali** model (doping dependent)
  - Integrating for 50 ns



- 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

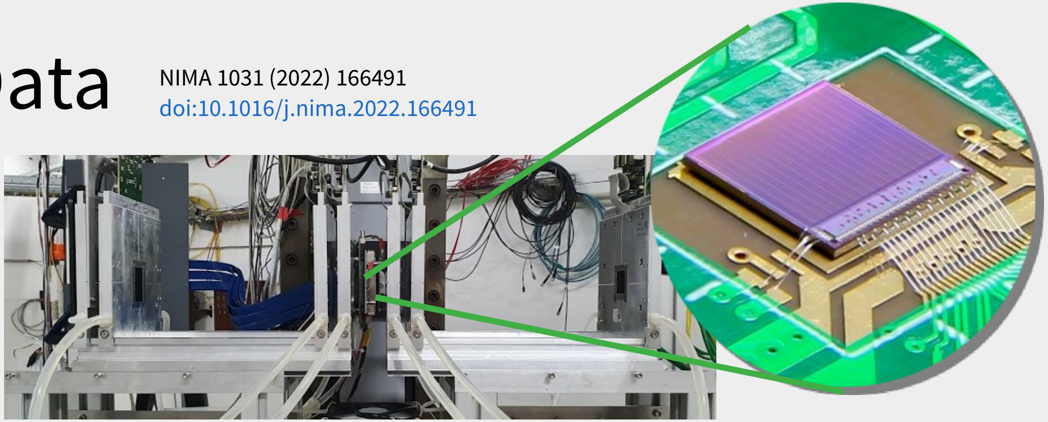


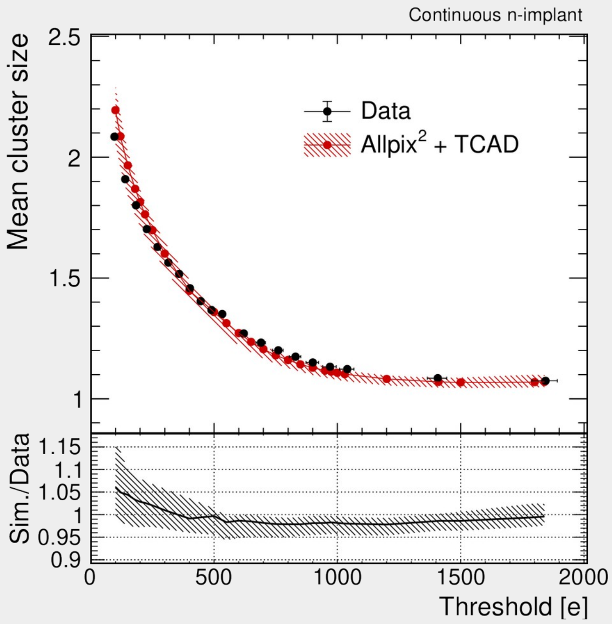
- Significant reduction of substrate contributions due to short lifetime in high-doping volume

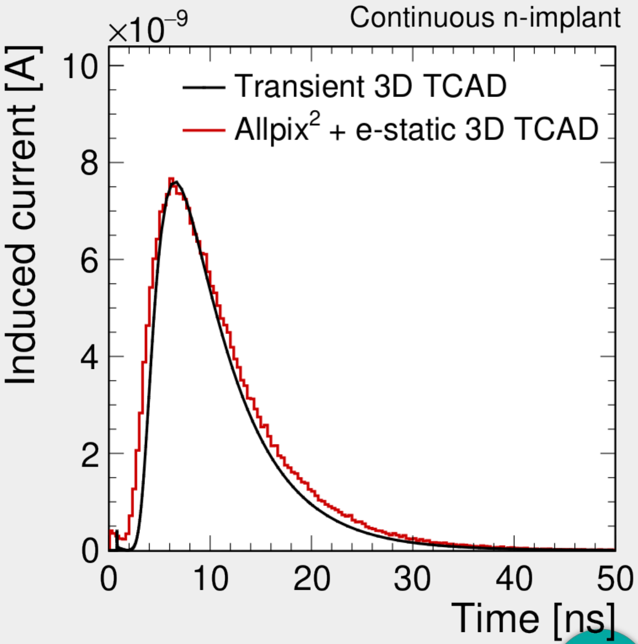
Comparison with Testbeam Data

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

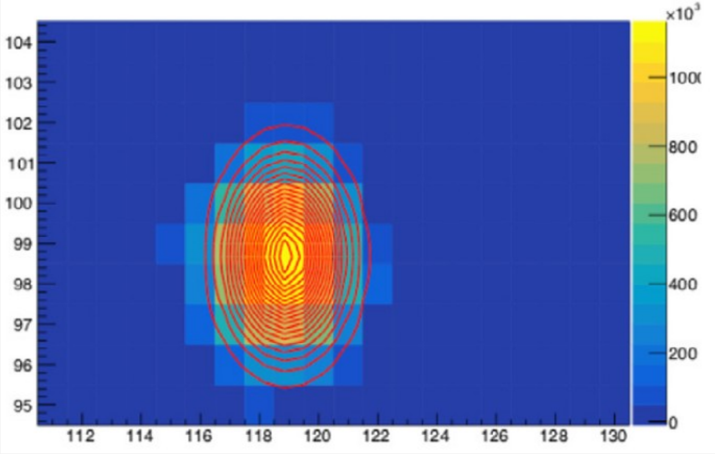






Machine Learning for Neutron Position Resolution

- 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



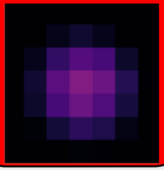
2D gaussian fitted to a UCN hit

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

Los Alamos NATIONAL LABORATORY

TEXAS The University of Texas at Austin

Input



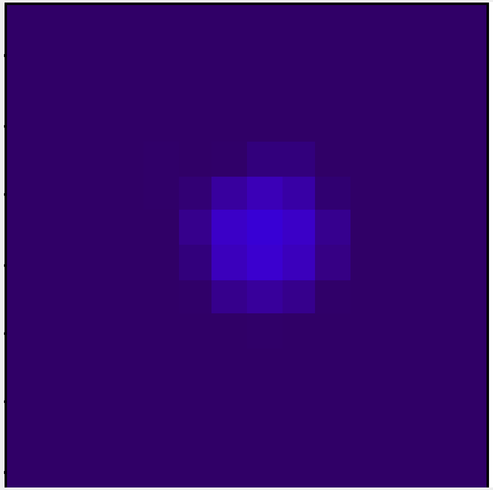
→ **Machine Learning Model** → **Output** Position Resolution

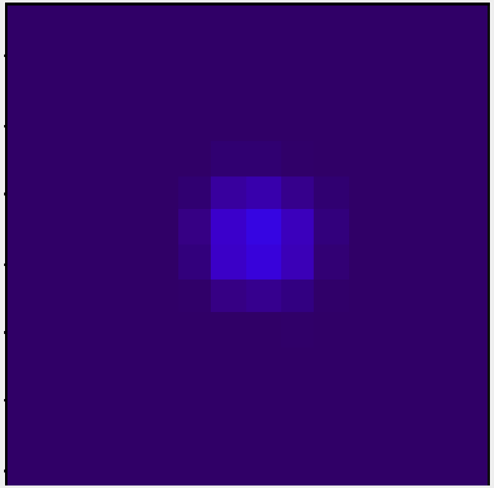
Allpix Squared for Neutron Imaging: Highlights

arXiv:2305.09562

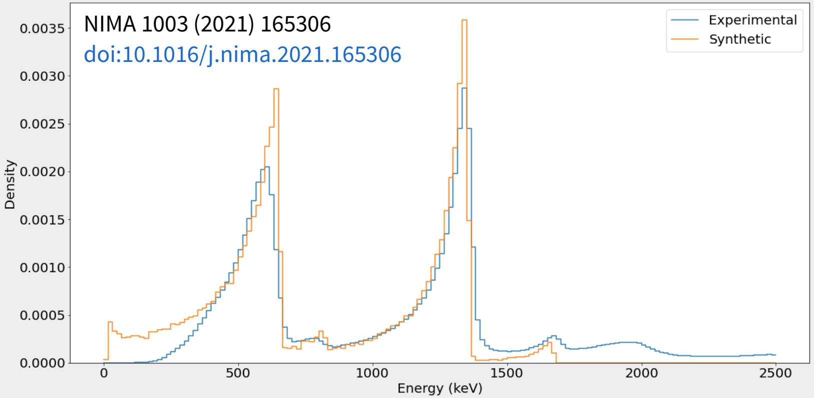
UCN Hit Images:

Experimental vs Allpix Squared





Experimental & simulated energy spectra



Summary

- Very successful development cycle of Allpix Squared 2.x
  - 5 feature releases 2.0 – 2.4, many additional patch releases
  - Many new features & effects added, extended simulation reach
  - Many very interesting applications – some presented in the coming days…

- Lots of development effort went into work towards APSQ 3.0
  – stay tuned for tomorrow!

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.