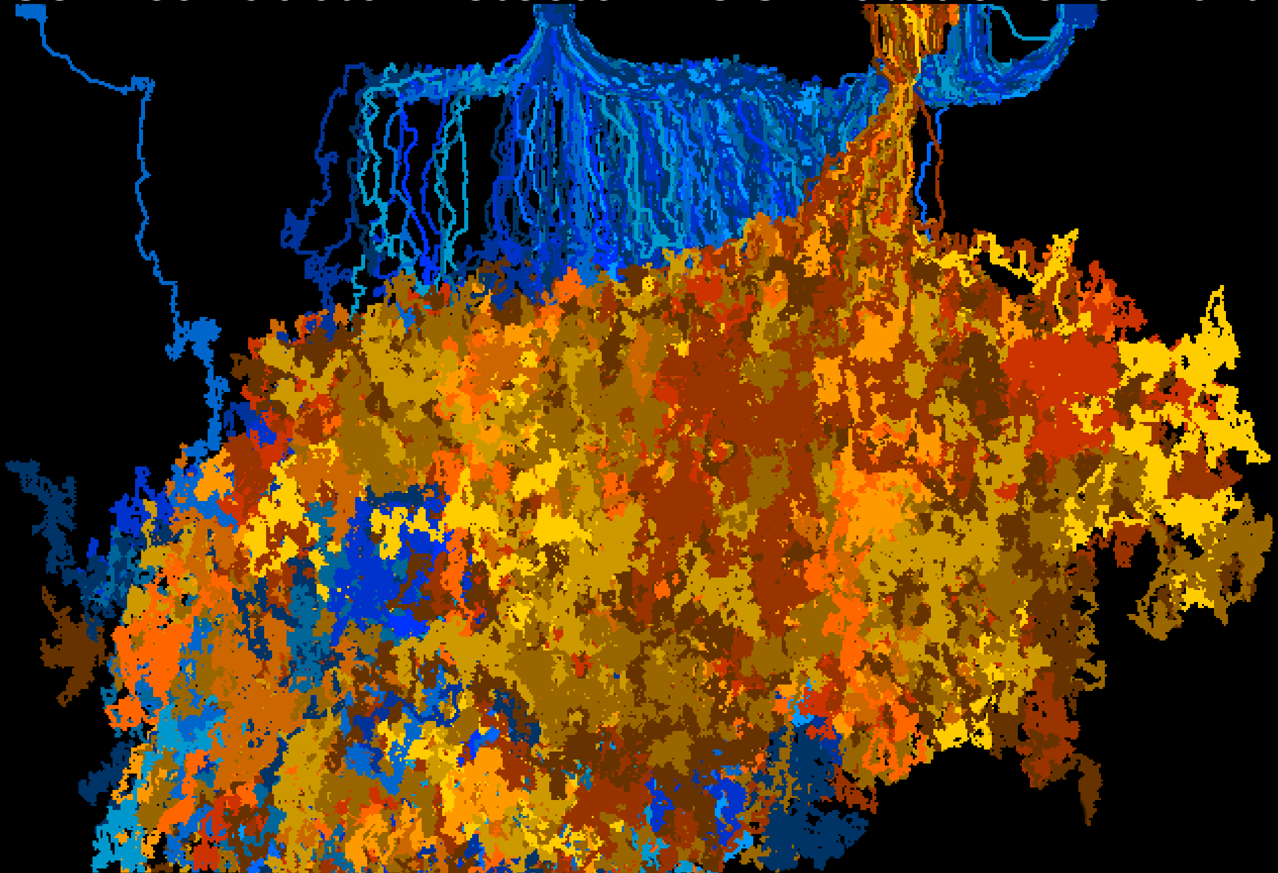
cern.ch/allpix-squared

Allpix Squared

Semiconductor Detector MC Simulations for Particle Physics and Beyond



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1st DRD3 Week, CERN
20 June 2024

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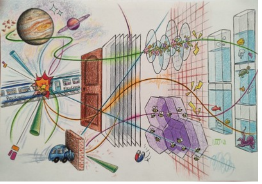


Semiconductor Detector MC Simulations

DRD3

Community Meeting 22-23/03/2023
Implementation of TF3
Solid State Detectors

- Complexity of detectors increases, more and more technologies available, different approaches combined (e.g. monolithic + LGAD)
  - Necessity of MC simulations growing
  - Some sensors / setups impractical to simulate in TCAD (time limitation, stochastics)
  - Community needs *common* flexible, tested & supported MC simulation tools

- 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

- Would be great to collate features in commonly maintained software (->SM)
  - Having several tools is valuable as testbed for algorithms
  - Well-maintained & supported common software will significantly ease use in community

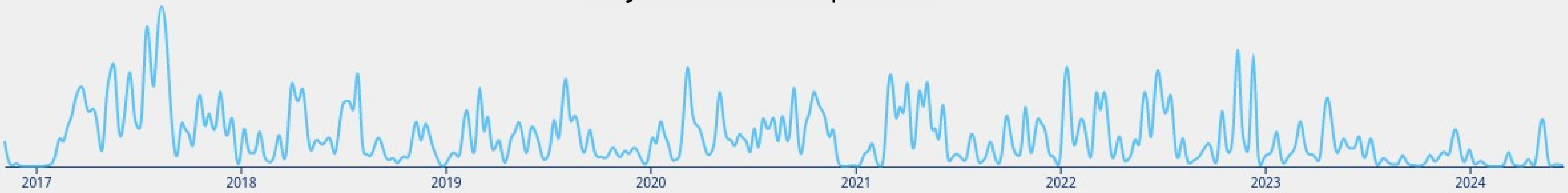
The Allpix² Framework

- Development of framework started within **CLICdp Collaboration**
- Now > 7 years of development with
  - 51 releases, current version 3.1.0
  - 5 user workshops
  - Close to 70 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

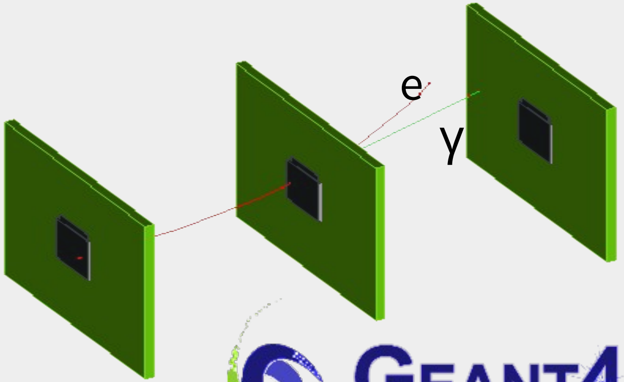
7 years of development



8882 commits | Last commit ≈ 4 days ago

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

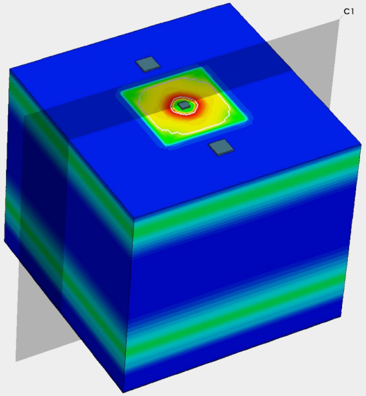


Geant4 – simulating interactions of particles passing through matter

- Detailed simulation of many interactions & processes
- Provide abstraction layer to auto-generate models and run simulation

TCAD – detailed simulation of field configuration, sensor behavior

- Tools & knowledge widely spread in community
- Provide possibility to import results to complement MC simulations



CRY – Cosmic-ray shower generator

HepMC3 – Reading HepMC event records from Event Generators

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
- So far 5 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

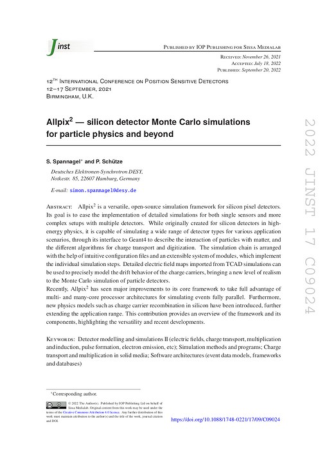
Combining TCAD and Monte Carlo methods to simulate CMOS pixel sensors with a small collection electrode using the Allpix² framework

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

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


Allpix²: Recent Developments and Applications

In preparation…


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

In preparation…

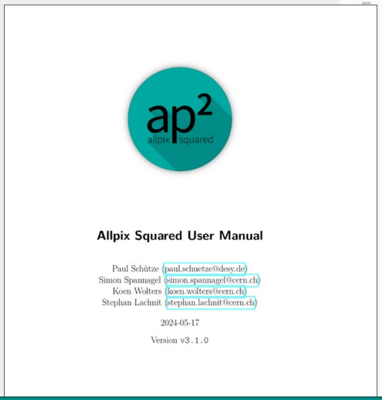
III. Low Entry Barrier for New Users

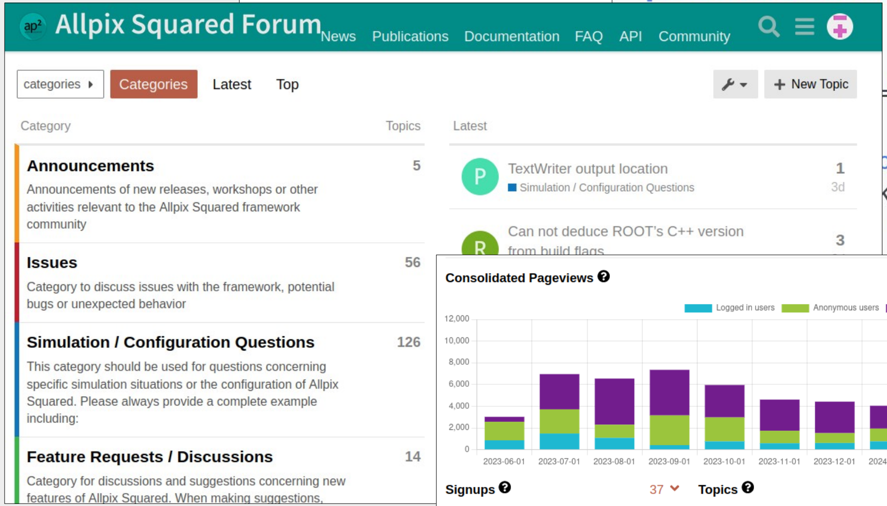
Simulation frameworks often very complex:
code complexity, lack of documentation, physics

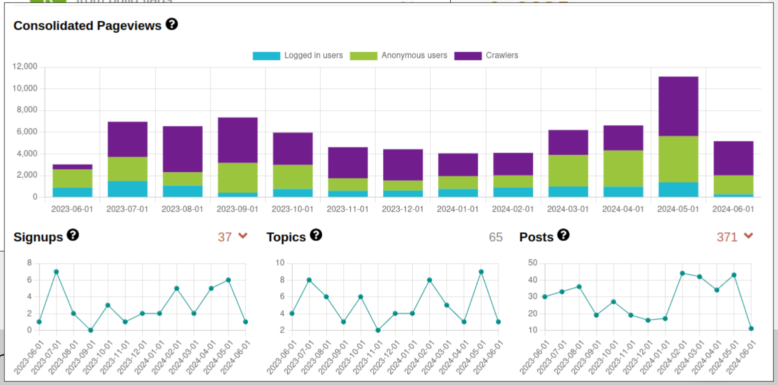
- Allpix Squared facilitates quick starts:
    - Extensive documentation / user manual
    - Public forum for help & exchange
    - Human-readable configuration files
    - Support for physical units
    - No coding or code-reading required

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

```
[AllPix]
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]
```

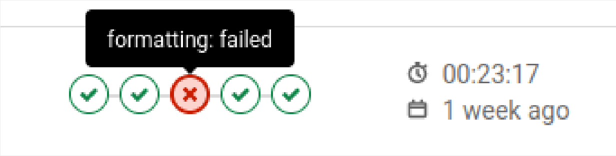






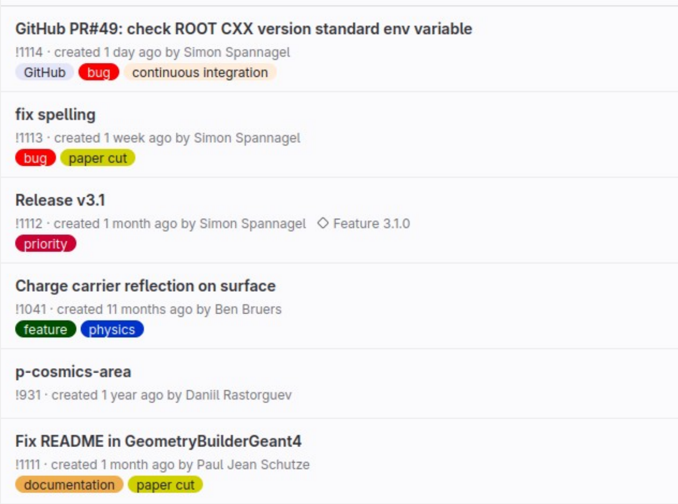
IV. Clean & Maintainable Code

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



Allpix Squared implements *best practices* for software development

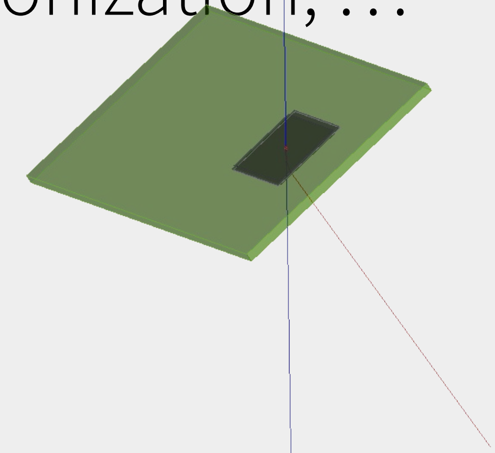
- Permissive MIT open-source license
- Semantic versioning (major.feature.patch)
- Extensive code reviews via merge requests
- Strict enforcement of coding conventions & formatting
- Regular static code analysis
- Following C++17 Standards



… see later for contribution cookbook

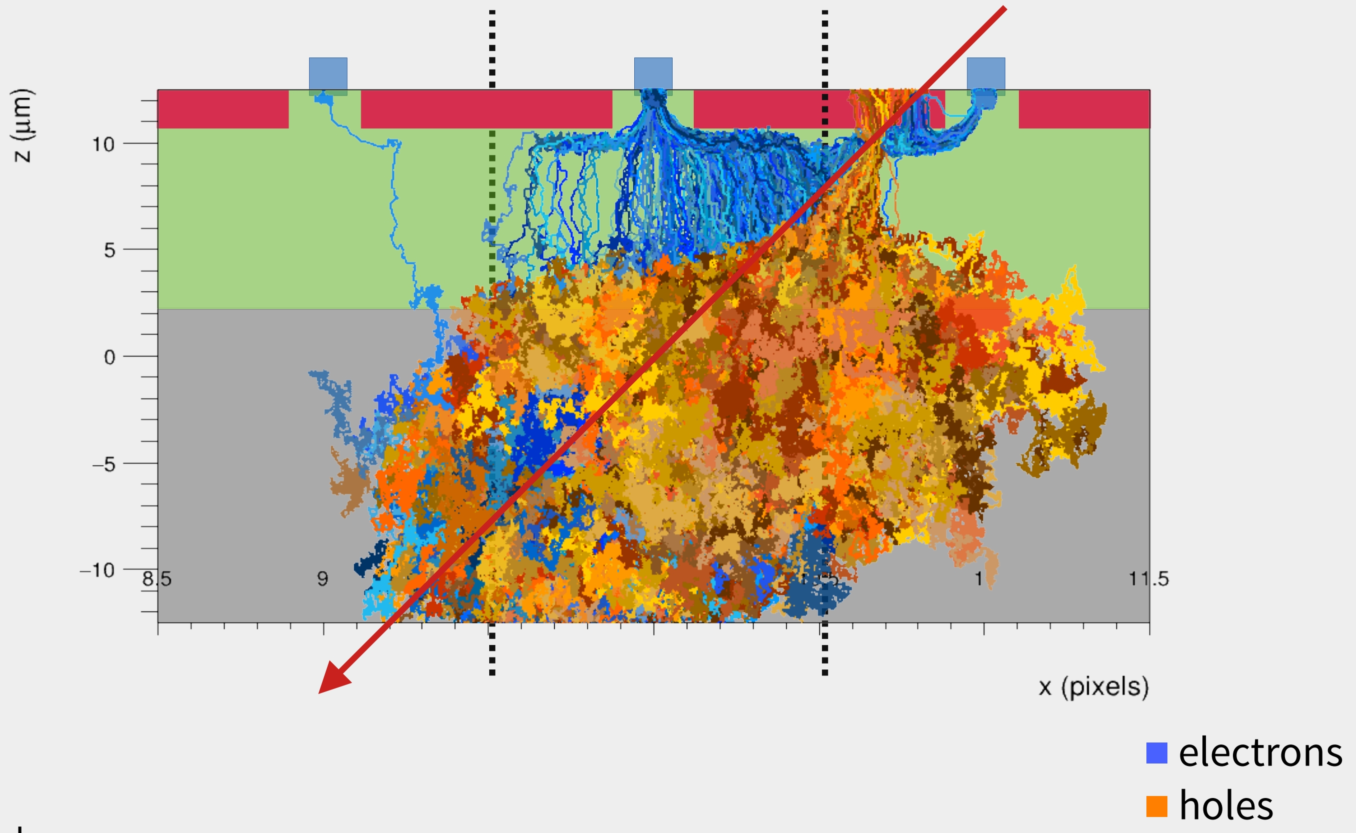
Some Application Highlights

MAPS, PET Scanners, 3D Sensors, Impact Ionization, …



Simulating a MAPS Sensor

- MIP entering sensor at 45deg
- 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

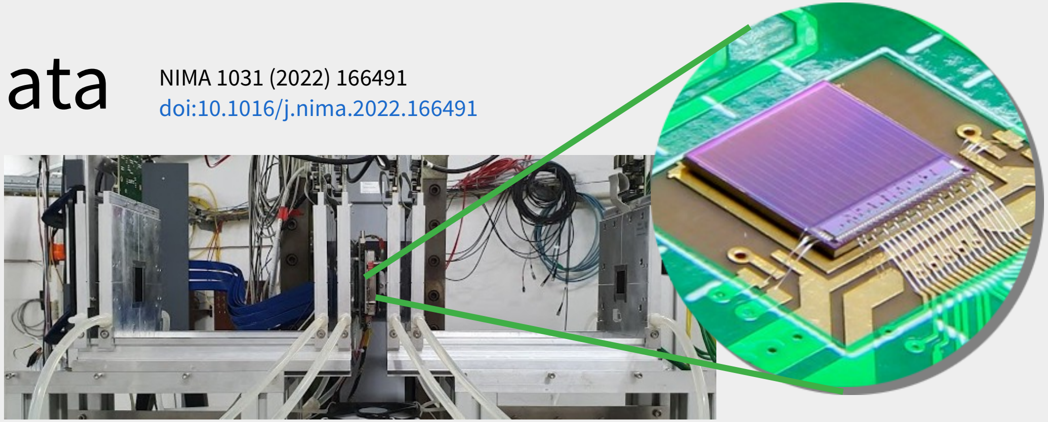


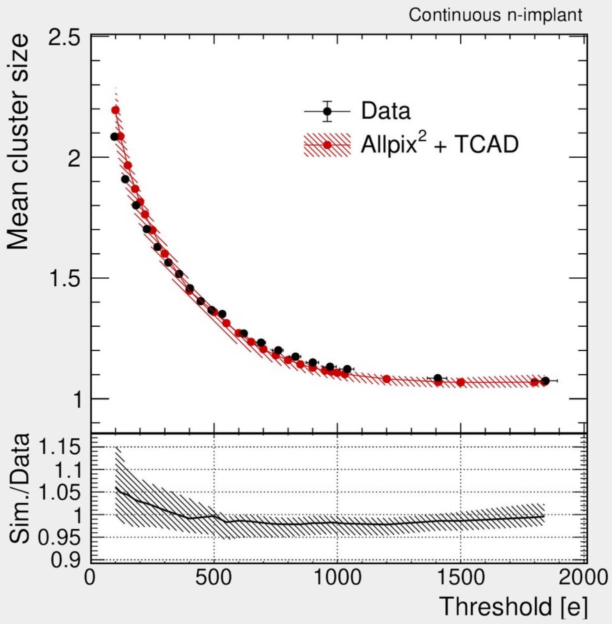
- Diffusion dominant in undepleted volume
- Carrier drift obeys sensor features (p-wells), collection at electrodes

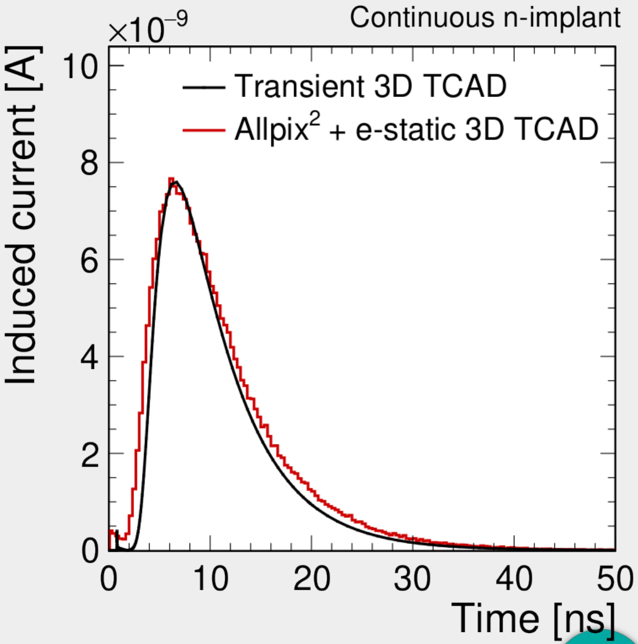
Comparison with Testbeam Data

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
- More MAPS simulation examples: Talk by Håkan Wennlöf



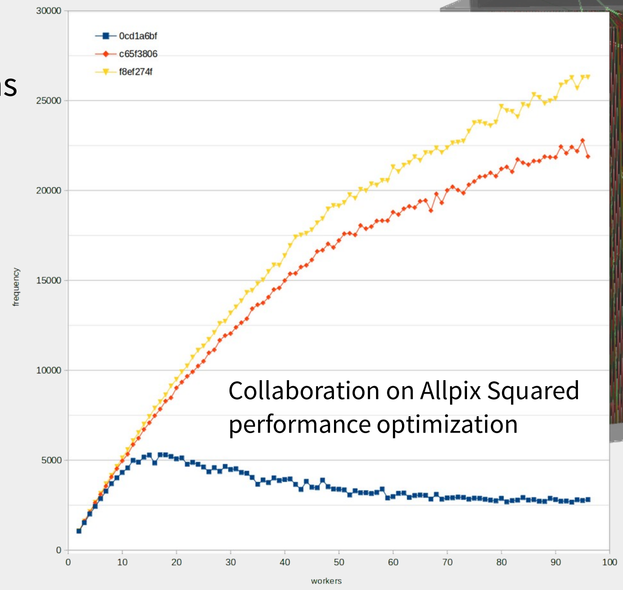


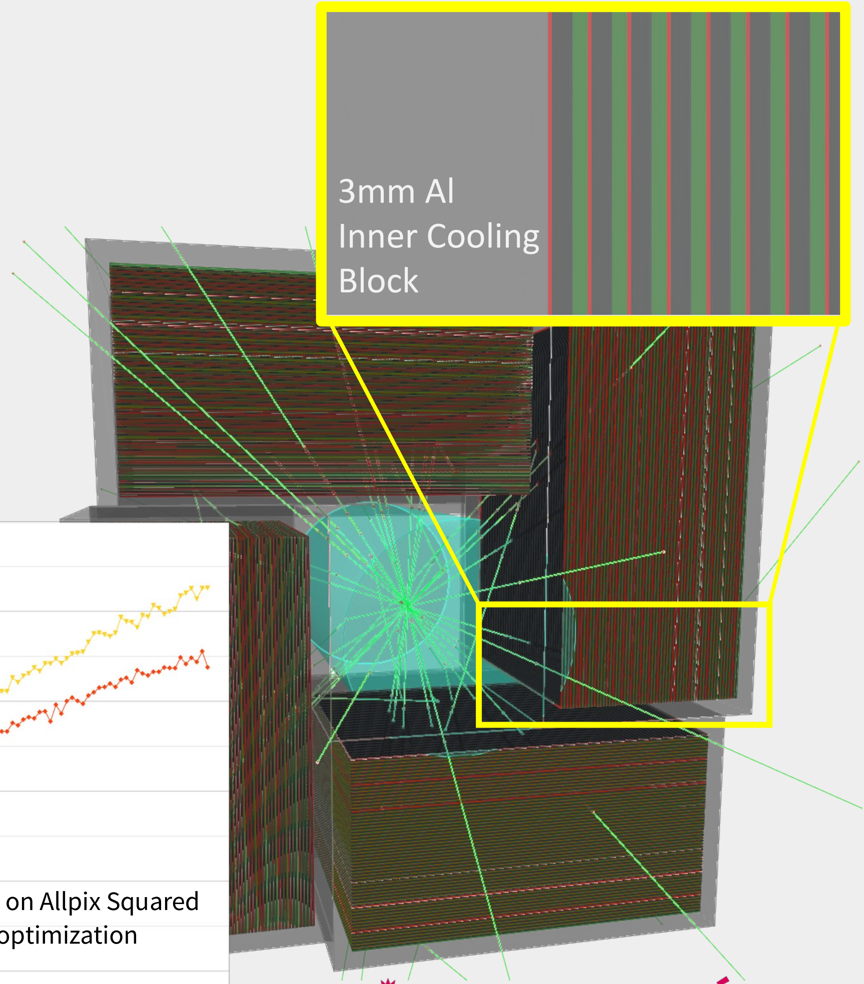


The 100µPET Project

New generation of PET scanners for high-res. molecular imaging
Talk by Mateus Vicente yesterday

- 4 Sectors, each 60 detection layers, monolithic Si sensors
- Simulating full setup with Allpix Squared
  - Script to generate geometry setup
    Placement of sensors, support, absorbers
  - Interaction from Geant4 module:
    Positron anni. 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^{10} events





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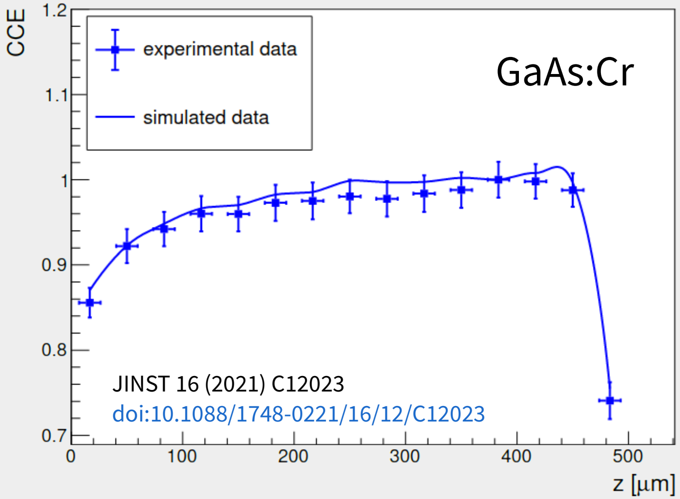
Non-Silicon Semiconductor Sensors

Allpix² supports a range of semiconductor materials:

- Selection of sensor material in det. model
- Definition of sensor materials impacts …
  - Material in Geant4 geometry
  - Charge carrier creation energy
  - Fano factor
  - Mobility model, recombination, …

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]

Example: Benchmark simulation using GaAs:Cr sensors,

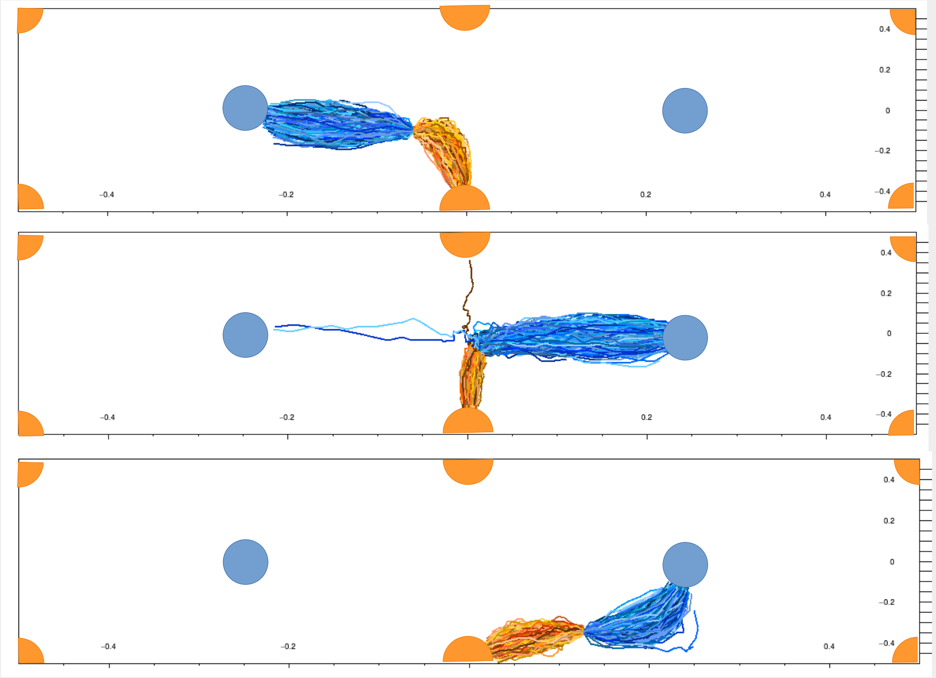


JINST 16 (2021) C12023
doi:10.1088/1748-0221/16/12/C12023

Simulation of 3D Sensors

- Definition of per-pixel implants via detector model
  - Position with respect to pixel center
  - Shape & orientation
  - 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
- 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



Impact Ionization

charge multiplication through impact ionization available

- Multiple models available, selection via configuration file:
  - Massey
  - van Overstraeten-de Man
  - Okuto-Crowell
  - Bologna
  - Optimized parameters for LGADs (RD50 work)
- Validation of algorithm, comparison of models e.g. in context of ATLAS HGTD

coefficient α and the length of the step l performed in the respective electric field. If the electric field strength stays below a configurable threshold E_{thr}, unity gain is assumed:

$$g(E,T) = \begin{cases} e^{l \cdot \alpha(E,T)} & E > E_{\text{thr}} \\ 1.0 & E < E_{\text{thr}} \end{cases} \quad (6.12)$$

The the following impact ionization models are available:

6.3.1 Massey Model

The Massey model [35] describes impact ionization as a function of the electric field E. The ionization coefficients are parametrized as

$$\alpha(E,T) = A e^{-\frac{B(T)}{E}}, \quad (6.13)$$

where A and $B(T)$ are phenomenological parameters, defined for electrons and holes respectively. While A is assumed to be temperature-independent, parameter B exhibits a temperature dependence and is defined as

$$B(T) = C + D \cdot T. \quad (6.14)$$

The parameter values implemented in Allpix² are taken from Section 3 of [35] as:

$A_e = 4.43 \times 10^5$ /cm $A_h = 1.13 \times 10^6$ /cm
$C_e = 9.66 \times 10^5$ V/cm $C_h = 1.71 \times 10^6$ V/cm
$D_e = 4.99 \times 10^2$ V/cm/K $D_h = 1.09 \times 10^3$ V/cm/K

d holes, respectively.

1 be selected in the configuration file via the parameter `multiplication_` `ey"`.

erstraeten-De Man Model

raeten-De Man model [36] describes impact ionization using Chynoweth's law,

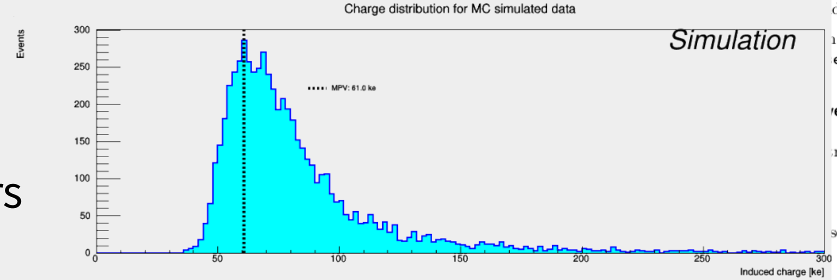
$$\alpha(E,T) = \gamma(T) \cdot a_\infty \cdot e^{-\frac{\gamma(T) \cdot b}{E}}, \quad (6.15)$$

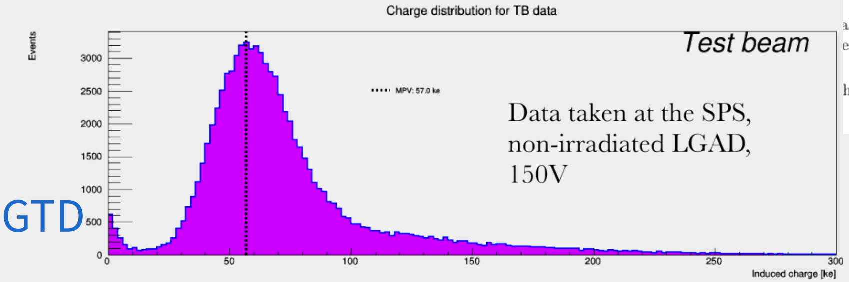
sets of impact ionization parameters $p = \{a_\infty, b\}$ are used depending on the

$$p = \begin{cases} p_{\text{low}} & E < E_0 \\ p_{\text{high}} & E > E_0 \end{cases} \quad (6.16)$$

aling of the ionization coefficient is performed via the $\gamma(T)$ parameter following entaurus TCAD user manual as:

$$h\left(\frac{0.063 \times 10^6\,\text{eV}}{28.6173 \times 10^{-5}\,\text{eV/K} \cdot T_0}\right) \cdot \tanh\left(\frac{0.063 \times 10^6\,\text{eV}}{28.6173 \times 10^{-5}\,\text{eV/K} \cdot T}\right)^{-1} \quad (6.17)$$





Contribute to the Development of Allpix Squared

How To Contribute – A Cookbook

- **Get in touch** – mail, forum, issue tracker, …
  Let’s discuss the idea, maybe we have input, maybe others are working on it already

- **Fork the repository**
  Creating your own copy of the code with which you can mess as much as you want

- **Start hacking**
  Implement the desired functionality, come back to us when you have doubts or questions

- **Make sure the CI passes**
  Enable the CI in your fork and publish your new code there – check that the CI works!

- **File a Merge Request**
  This provides us a central point to discuss and review all your code changes

- **See your code being merged and published!**

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, simulate, contribute, share!

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.