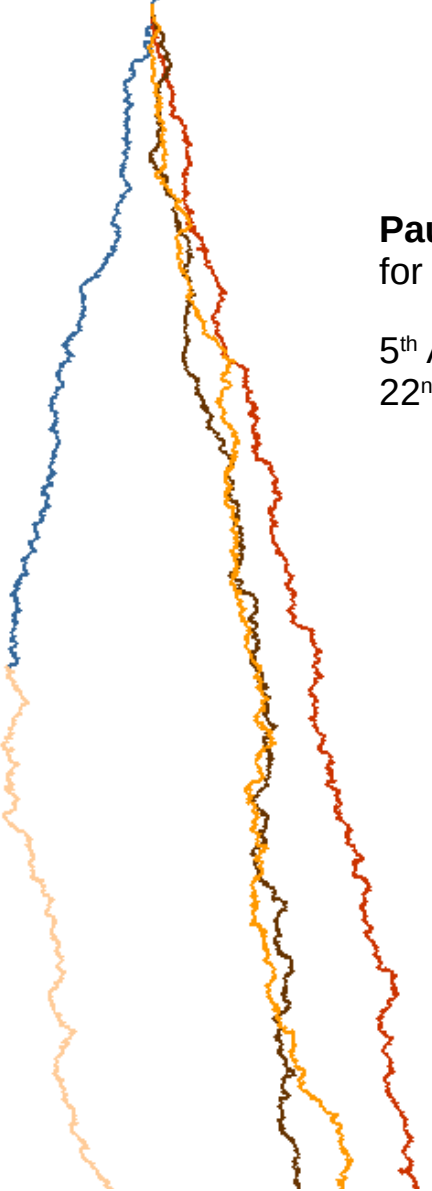
Allpix Squared

What's new?



Paul Schütze
for the Allpix Squared Authors

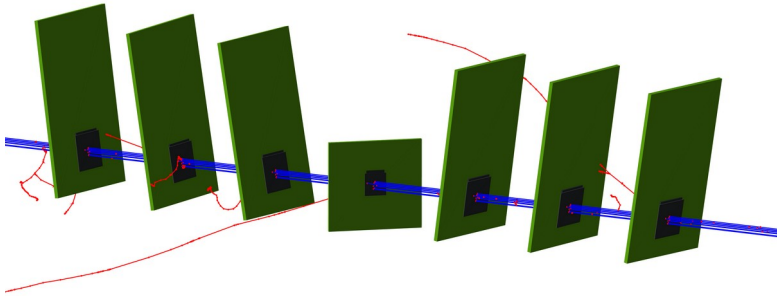
5th Allpix Squared User Workshop
22nd May 2024

- Paul Schütze, DESY
- Simon Spannagel, DESY
- Mohamed Moanis Ali, GSOC2019 Student
- Jay Archer, University of Wollongong
- Mathieu Benoit, BNL
- Thomas Billoud, Université de Montréal
- Tobias Bisanz, CERN
- Bogdan-Mihail Blidaru, Heidelberg University
- Sebbe Blokhuizen, Stockholm University, Sioux Technologies
- Marco Bomben, Université de Paris
- Koen van den Brandt, Nikhef
- Ben Bruers, DESY
- Carsten Daniel Burgard, DESY
- Maximilian Felix Caspar, DESY
- Liejian Chen, Institute of High Energy Physics Beijing
- Naomi Davis, DESY
- Manuel Alejandro Del Rio Viera, DESY
- Malinda de Silva, DESY
- Katharina Dort, University of Gießen
- Neal Gauvin, Université de Genève
- Yajun He, DESY
- Ryan Heller, LBNL
- Lennart Huth, DESY
- Daniel Hynds, University of Oxford
- Francisco-Jose Iguaz-Gutierrez, Synchrotron SOLEIL
- Maoqiang Jing, Institute of High Energy Physics Beijing
- Moritz Kiehn, Université de Genève
- Rafaella Eleni Kotitsa, CERN
- Stephan Lachnit, DESY
- Hugo Natal da Luz, Czech Technical University in Prague
- Salman Maqbool, CERN Summer Student
- Stefano Mersi, CERN
- Ryuji Moriya, CERN Summer Student, University of Glasgow
- Sebastien Murphy, ETHZ
- Andreas Matthias Nürnberg, KIT
- Sebastian Pape, TU Dortmund University
- Marko Petric, CERN
- Florian Michael Pitters, HEPHY
- Radek Privara, Palacky University Olomouc
- Renato Quagliani, CERN
- Nashad Rahman, The Ohio State University
- Sabita Rao, GSDocs2020 Student
- Daniil Rastorguev, DESY
- Edoardo Rossi, DESY
- Sara Ruiz Daza, DESY
- Jihad Saidi, Université de Genève
- Andre Sailer, CERN
- Tasneem Saleem, Synchrotron SOLEIL
- Arka Santra, Weizman Institute
- Christian Scharf, HU Berlin
- Enrico Jr. Schioppa, Unisalento and INFN Lecce
- Sebastian Schmidt, FAU Erlangen
- Sanchit Sharma, Kansas State University
- Xin Shi, Institute of High Energy Physics Beijing
- Petr Smolyanskiy, Czech Technical Univbersity Prague
- Viktor Sonesten, GSOC2018 Student
- Reem Taibah, Université de Paris
- Ondrej Theiner, Charles University
- Annika Vauth, University of Hamburg
- Mateus Vicente Barreto Pinto, CERN
- Håkan Wennlöf, DESY
- Andy Wharton, Lancaster University
- Morag Williams, University of Glasgow
- Koen Wolters
- Samuel Wood, University of Oxford

Motivation & History

Initial Motivation: **Monte Carlo simulation of silicon pixel detectors!**

- Started at CERN EP-LCD – different groups from High Energy Physics got involved
  - ➔ Different phases of detector R&D to cover
  - Required a tool that at the same time is useful for …
    - Generic sensor R&D
    - Integration of detector systems, e.g. test beam setups
    - Validating simulation algorithms

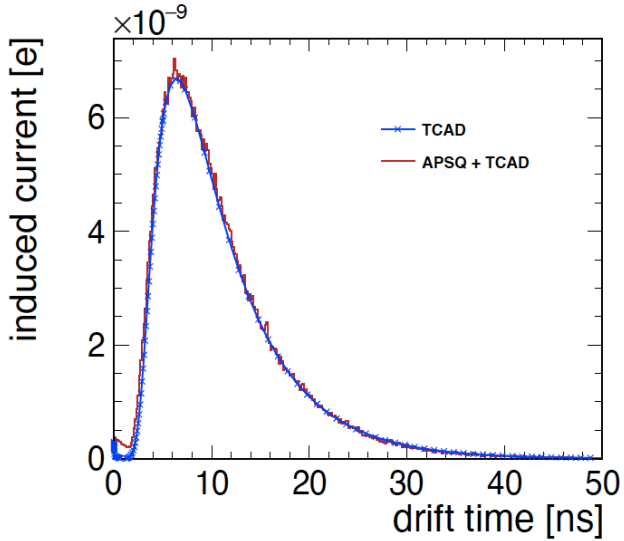


- ➔ Sep. 2017: Allpix Squared 1.0 released with modular design & basic set of modules

Motivation & History

The devil's in the details:
HEP community targets high-precision simulations & realistic behaviour

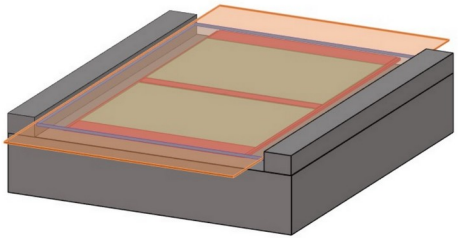
- Access to time-resolved information
  - ➔ Transient simulation, pulse storage, amplifier simulation …
- Implementation of further physics effects
  - ➔ User-selected recombination, mobility and trapping models, impact ionisation, Shockley-Ramo theorem …
- Interfaces to other frameworks
  - ➔ Import TCAD electric fields, weighting potentials

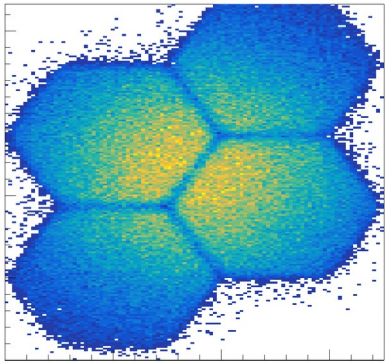


Motivation & History

The more the merrier:
New users & applications – many of them outside the HEP community

- Demands interfaces to other software and frameworks
  - ➔ Charge carrier input from file, different particle sources, flexible G4 interface
  - ➔ Various output formats, storage options, interfaces to analysis frameworks
- Different detector types & geometries
  - ➔ Monolithic & hybrid sensors, radial strips, 3D pixels, hexagonal pixels …
- Different detector materials
  - ➔ Sensor material as a simulation parameter
- Various applications
  - ➔ Passive materials, magnetic field, cosmic rays, …



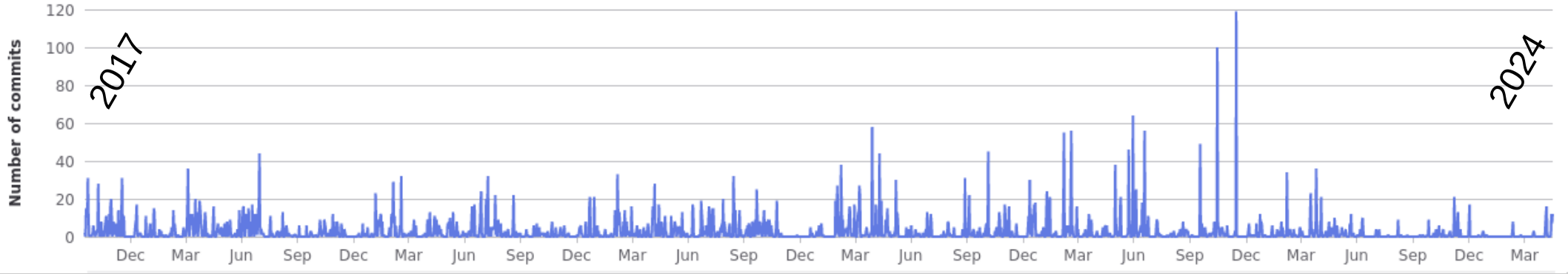


The Allpix² Framework

- Development of new framework started within CLICdp Collaboration
  - Now **7 years** of development with …
  - **54 releases**
  - **5** user **workshops** (as of now)
  - **77** code **contributors**

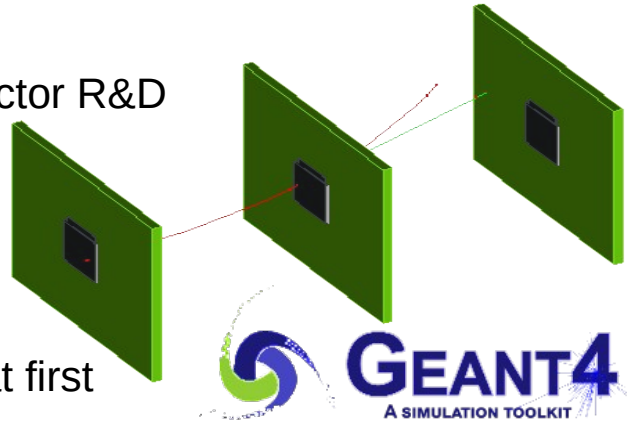
Development based on four principles:

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

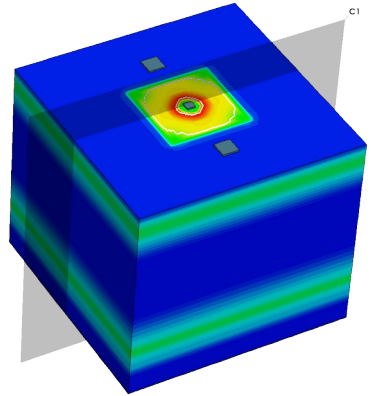


Geant4 – simulating interactions of particles passing through matter

- 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

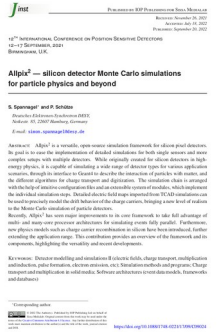
- Detailed understanding of field configuration, sensor behavior
- Tools & knowledge widely spread in community
- Provide possibility to import results to complement MC simulations



II. Well-Tested & Validated Algorithms

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

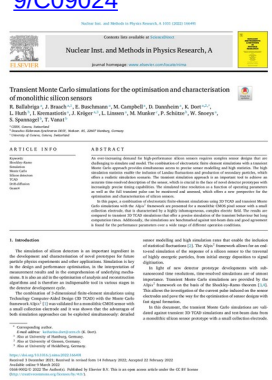
- Validation of algorithms is a crucial and time-consuming process
- User workshops for exchange of the community, discussions, planning…
- Validating as much as possible against data
- Publishing reference studies including full simulation configuration used
- Providing automated tests for every new feature



JINST 17 (2022) C09024
doi:10.1088/1748-0221/17/9/C09024

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

III. Low Entry Barrier for New Users

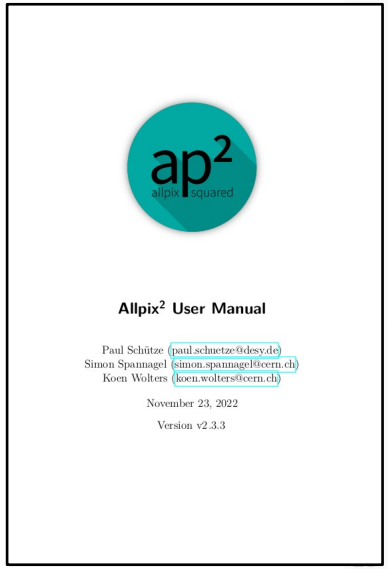
Simulation frameworks are often very complex: code complexity, lack of documentation, physics

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

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

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

[SimpleTransfer]
```

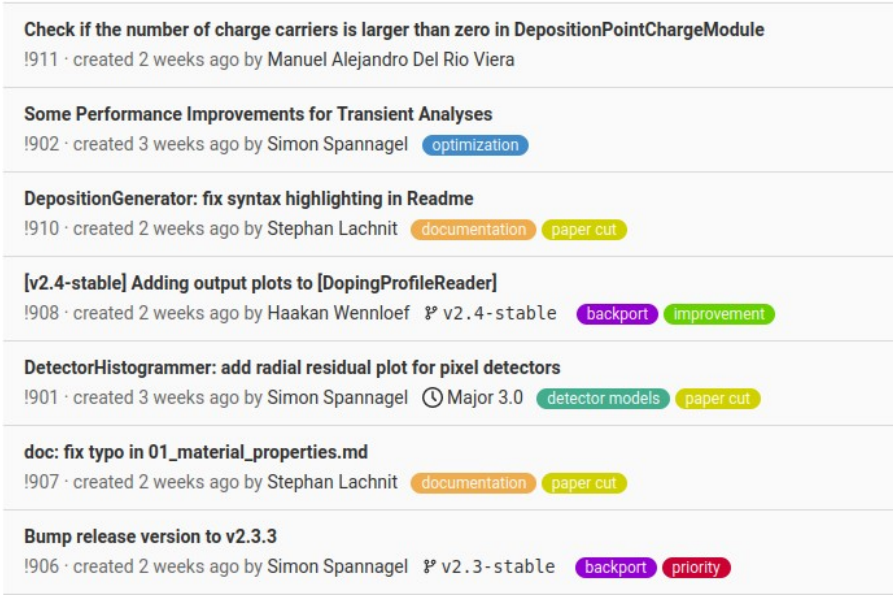
bcgs
Bonn-Cologne Graduate School of Physics and Astronomy

IV. Clean & Maintainable Code

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

Allpix Squared implements best practices for software development

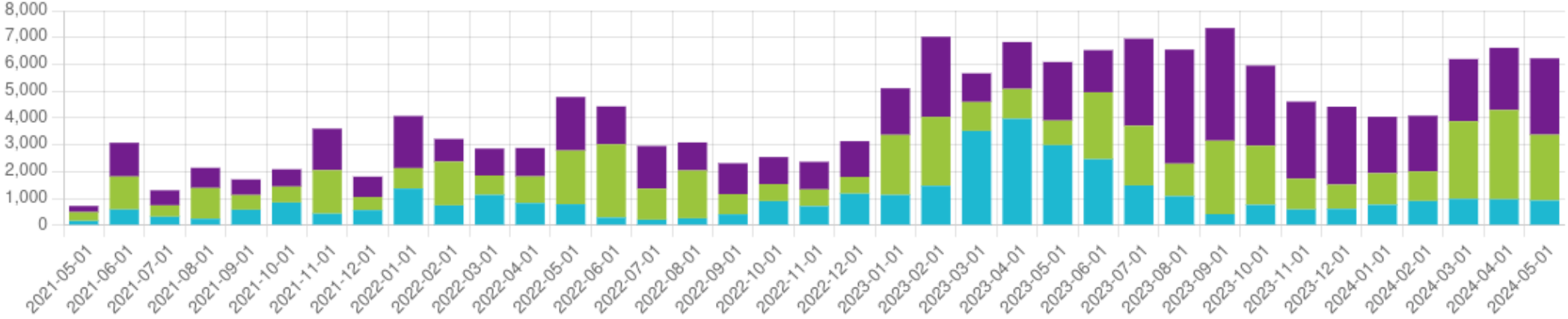
- Permissive MIT open-source license
- Semantic versioning (major.feature.patch)
- Extensive code reviews via merge requests
- Strict enforcement of coding
- conventions & formatting
- Regular static code analysis
- Following C++17 Standards



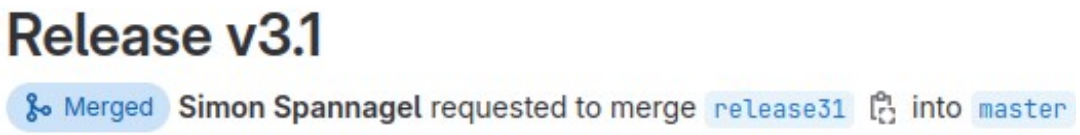
The Community – Forum

- Increasing activity in the forum
- Please share your experience with other users

Pageviews



Allpix Squared v3.1



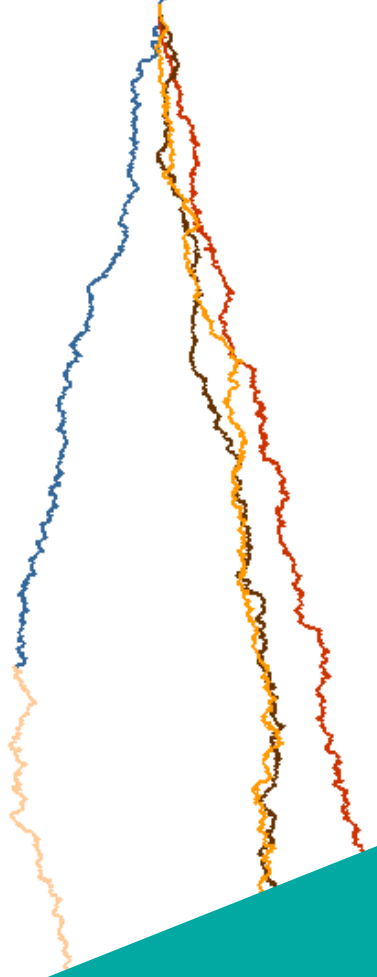
Since v3.0:

403 commits

19 contributors

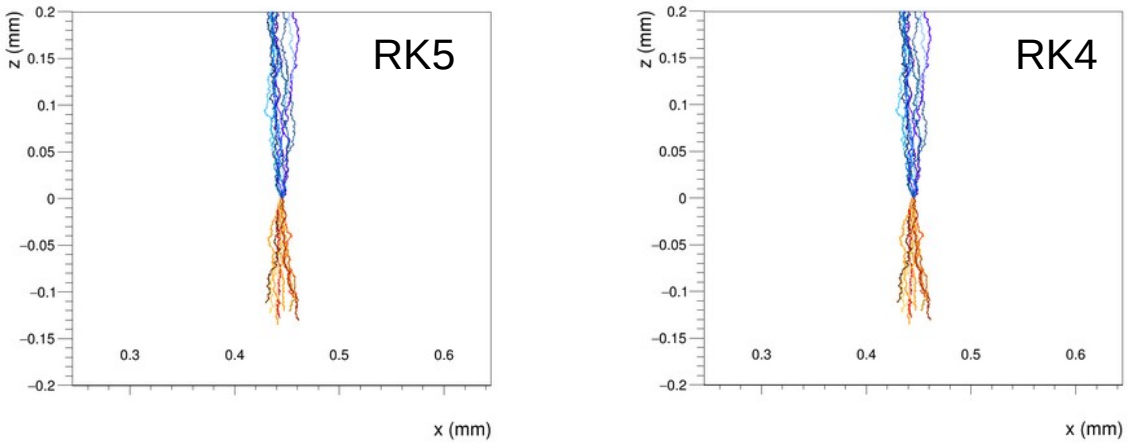
14 new contributors

Charge Carrier Propagation

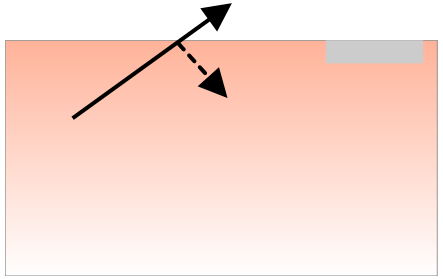


Propagation (Generic & Transient) !1035, !1043

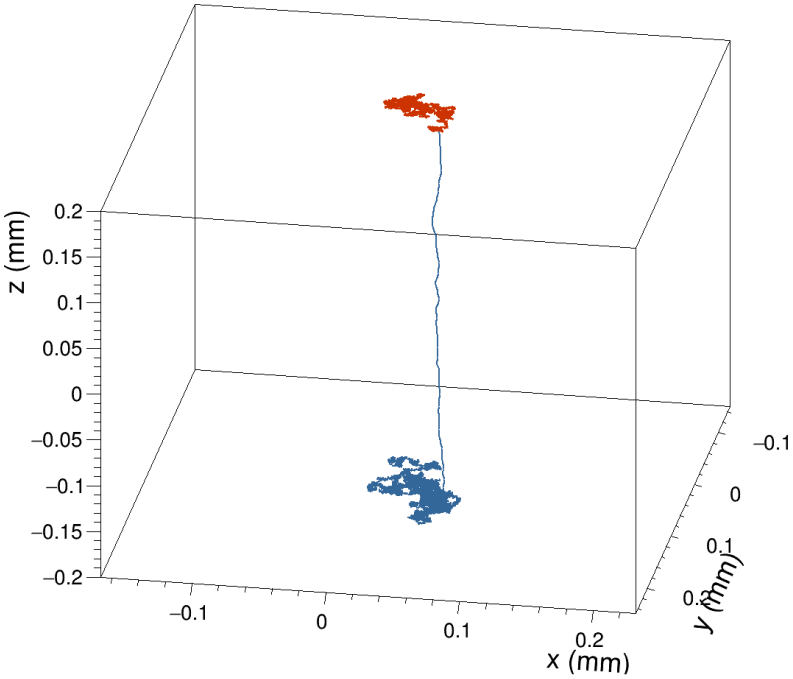
- Diffusion determined based on pre-step field and doping (was: post-step)
  - ➔ Prevents zero-diffusion in case of single-step propagation
- Placement of charge carriers at sensor boundary or implant intercept *before* determination of recombination, trapping and impact ionisation
  - ➔ Impact ionisation and trapping only calculated when carrier is not *HALTED* (end of propagation)
- Change default Runge-Kutta tableau for *TransientPropagation* to fourth-order RK



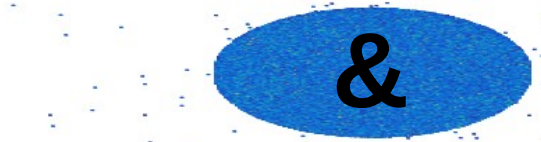
Charge Carrier Reflection !1041



- Charge carriers can be reflected at the sensor boundaries along *z*
  - New parameter: *surface_reflectivity*, ranging from …
    - 0.0 – no reflectivity (default) to …
    - 1.0 – full reflectivity
  - When charge carrier leaves sensor along *z,* it is relocated in *z*
  - Reflection only when charge carrier is outside implant
  - Stop propagation (state *HALTED*) when sensor was left in the transverse



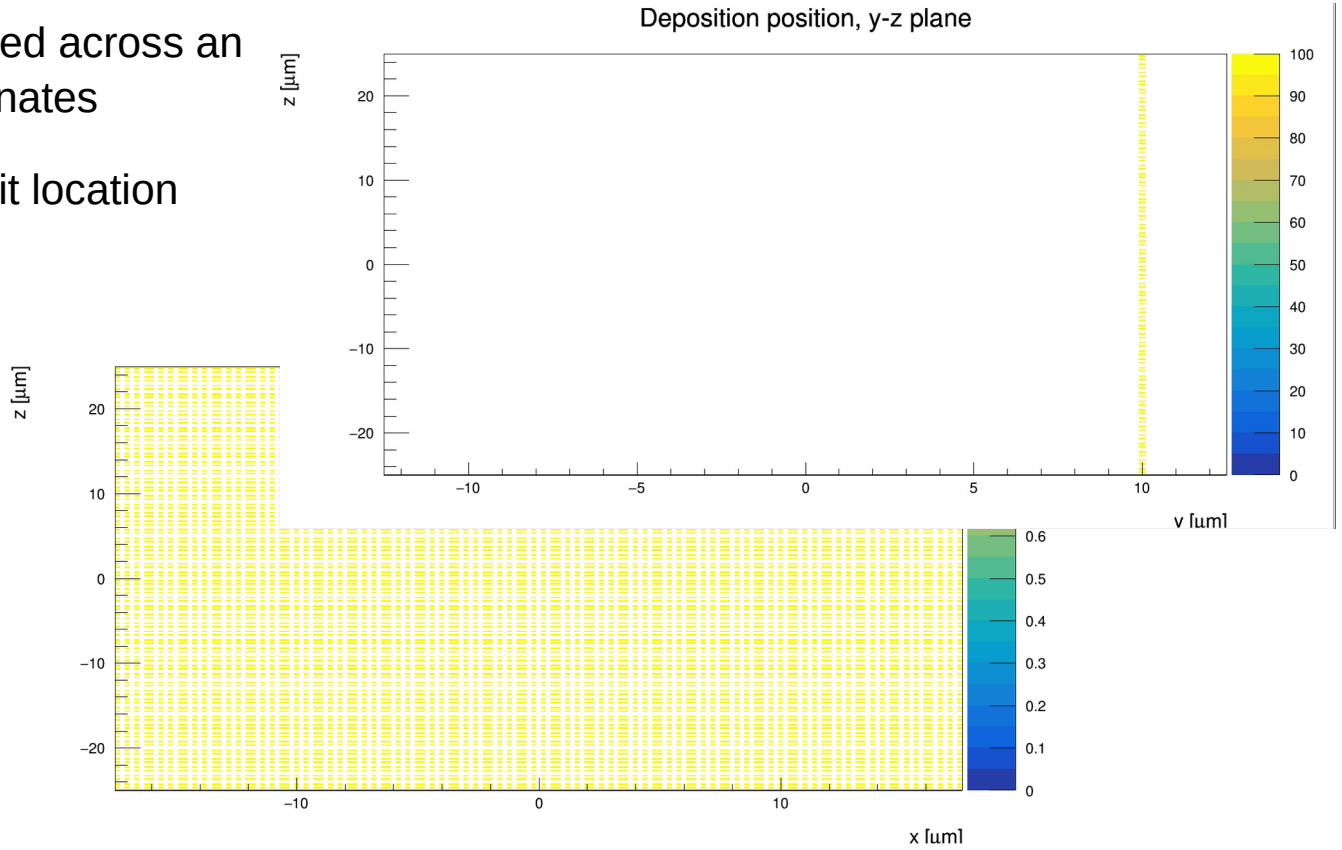
Charge Deposition



Geant4

DepositionPointCharge: Deposit Scan in 1D & 2D !1084

- Depositions can now be scanned across an arbitrary combination of coordinates
- Event-by-event offset of deposit location

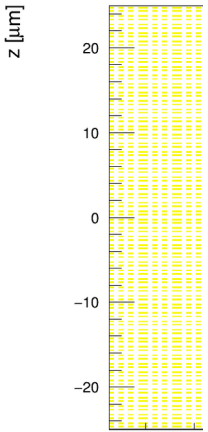


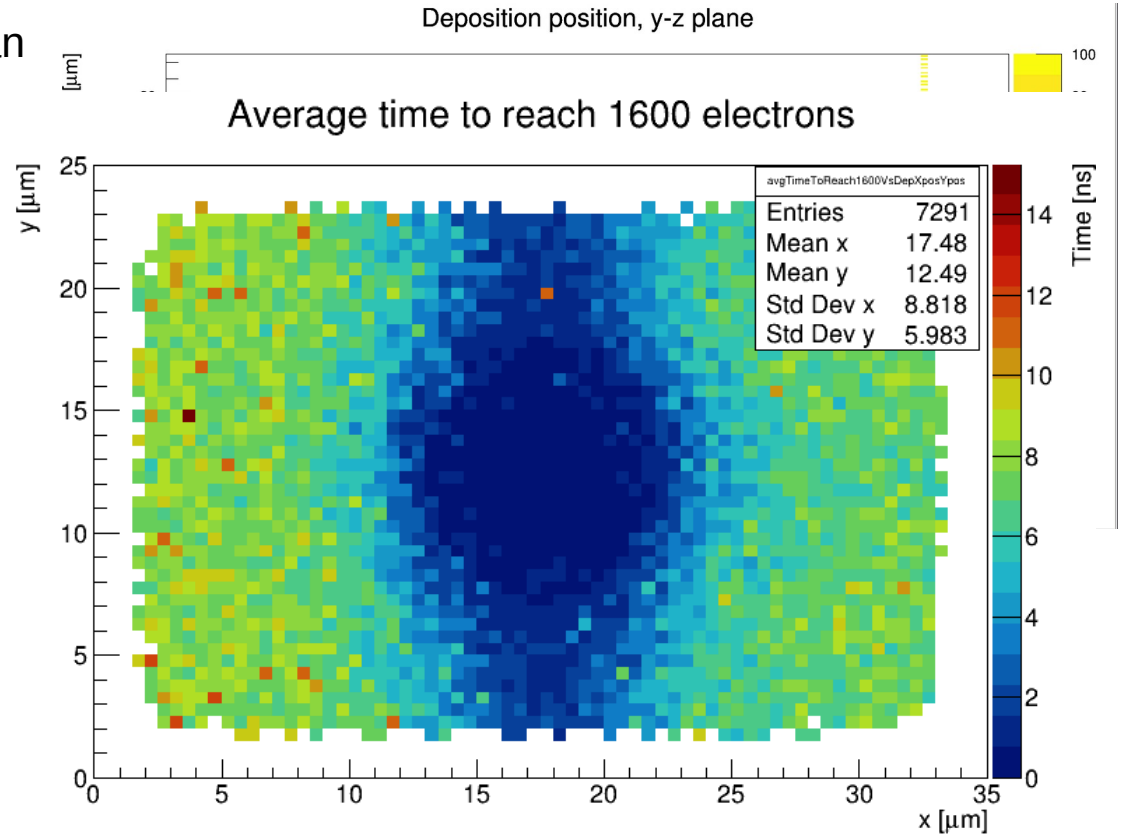

```
[DepositionPointCharge]
source_type = "point"
model = "scan"
scan_coordinates = x z
position = 0um 10um 0um
number_of_charges = 1000
output_plots = true
output_plots_bins_per_um = 5
```

DepositionPointCharge: Deposit Scan in 1D & 2D !1084

- Depositions can now be scanned across an arbitrary combination of coordinates
- Event-by-event offset of deposit location
- E.g. create “collection time” maps

```
[DepositionPointCharge]
source_type = "point"
model = "scan"
scan_coordinates = x z
position = 0um 10um 0um
number_of_charges = 1000
output_plots = true
output_plots_bins_per_um = 5
```

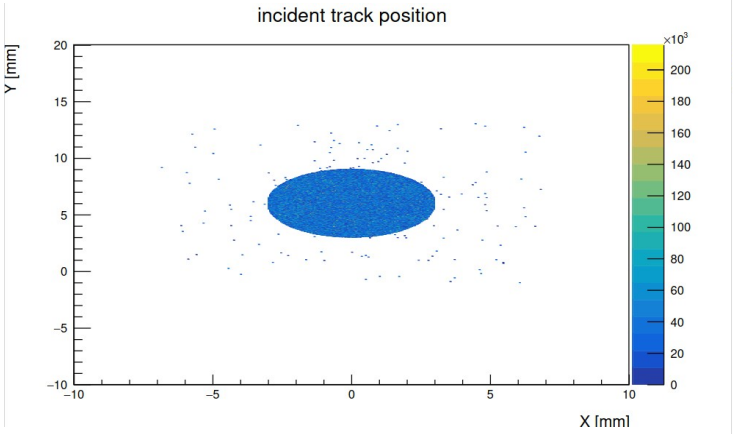


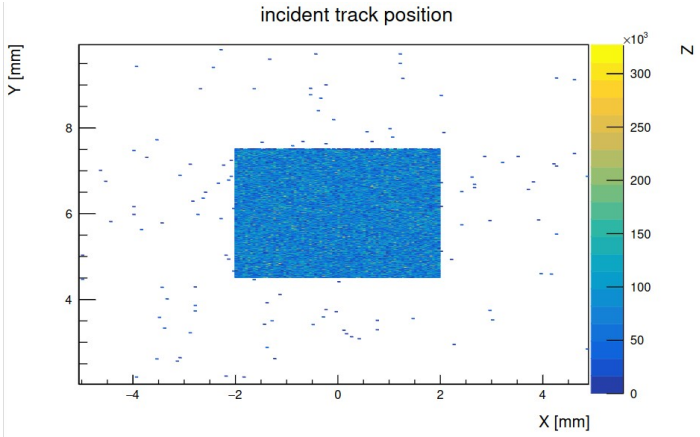


Beam Me Up! But stay focussed. Or rectangular. Or elliptical. !1077 & !1104

- Source type *beam* can have a focal point (see talk by Malinda, Thursday):
  - New parameter *focus_point*, *m*utually exclusive with *beam_divergence* parameter
- Rectangular and elliptical shapes added for source type *beam*
  - Key *beam_size* can take one (square / round) or two values (rectangular / elliptical)
  - Reproduce collimated beams or trigger geometries

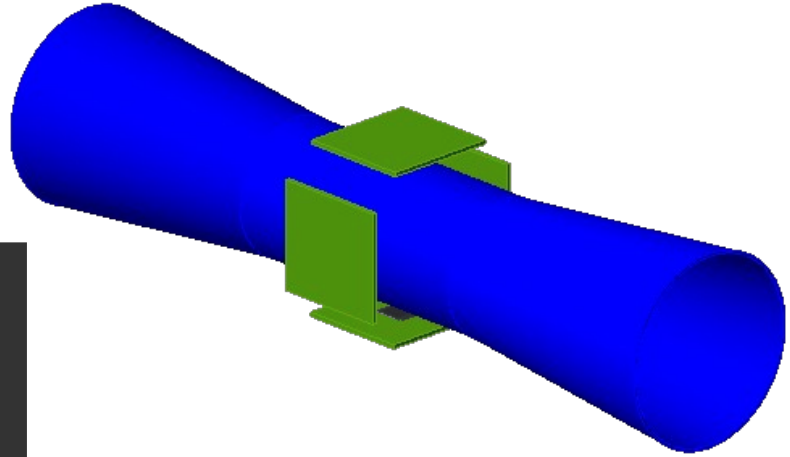
```
[DepositionGeant4]
source_type = "beam"
flat_beam = true
particle_type = "e-"
source_energy = 5GeV
beam_size = 3mm 4mm
beam_shape = Rectangle
beam_direction = 0 0 1
model = "fixed"
```





Cones !1110

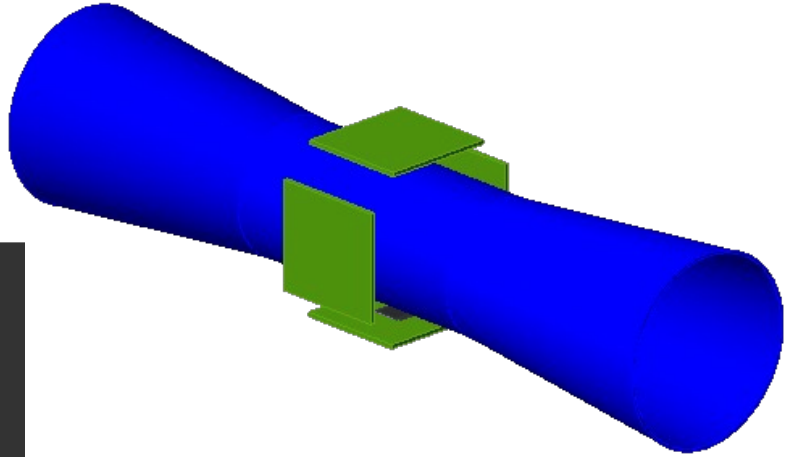
- Introduced cones as passive material model
  - Inner and outer radii at begin and end configurable
  - Partial cones possible
  - Create beam pipes

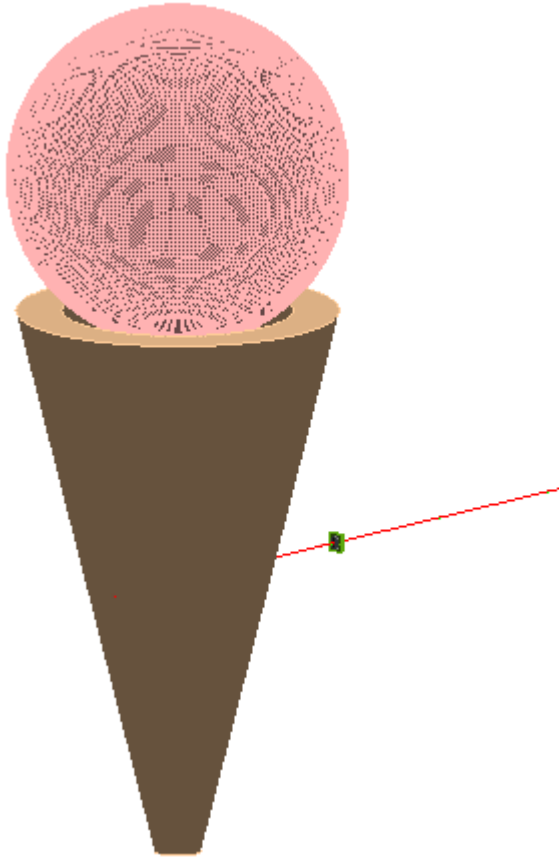


```
[cone1]
type = "cone"
outer_radius_end = 10mm
inner_radius_end = 9mm
outer_radius_begin = 20mm
inner_radius_begin = 9mm
starting_angle = 0deg
arc_length = 180deg
length = 30mm
position = 0 0 10mm
orientation = 0 0 0
material = "beryllium"
role = "passive"
```

Cones !1110

- Introduced cones as passive material model
  - Inner and outer radii at begin and end configurable
  - Partial cones possible
  - Create beam pipes
  - … or others





```
[cone1]
type = "cone"
outer_radius_end = 10mm
inner_radius_end = 9mm
outer_radius_begin = 20mm
inner_radius_begin = 9mm
starting_angle = 0deg
arc_length = 180deg
length = 30mm
position = 0 0 10mm
orientation = 0 0 0
material = "beryllium"
role = "passive"
```

Geant4 Physics Lists !1095

- Status Quo:
  - Only Geant4 standard physics lists are available through Allpix Squared
- Now:
  - Frame for additional physics lists set
  - Added *MicroElec* physics list (improved spatial resolution for silicon)

Geant4 – Unphysical Events catch them if you can !1053

- Unphysical events observed during Geant4 execution:
  - Massive step of negative length – followed by particle being “stuck” and infinity run time
- Solved by adding a *G4StepHook* and aborting events when a negative step length is observed

```
(E) (E: 7312) [Geant4] Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
(E) (E: 7312) [Geant4]     0   -0.103    0.037    0.183      6.98        0        0         0       World initStep
(E) (E: 7312) [Geant4]     1 2.41e+22 9.48e+20 4.46e+20      6.98        0 -2.41e+22 -2.41e+22       World hIoni
(W) (E: 7312) [R:DepositionGeant4] Negative step length found; aborting event.
```

➔ Small performance impact expected – basically a “G4UnphysicalEvent insurance”

Performance

Function / Call Stack	CPU Time ▼
__pow	22.995s
allpix::DetectorField<ROOT::Math::DisplacementVector3D<ROOT::Math::Cartes	3.888s
std::mersenne_twister_engine<unsigned long, (unsigned long)64, (unsigned long)	3.347s
operator()	3.213s
llround	2.930s

Field Lookup & Coordinate Transformations

!1011

!1009

- Reduce computation during field lookup to the minimum possible
  - Introduce *FieldType::CUSTOM1D* for custom fields only dependent on z
  - Check field type before performing non-required calculations
  - Benchmarks:
    - Transient MAPS simulation (e-field, doping, weighting potential all maps): 24% speedup
    - *test_performance/test_03-multithreading* (single-threaded): 20%
- In several locations, simple checks can prevent costly coordinate transformations …
  - When we have no implants configured, we don't need to do a coordinate transformation
  - When we have SENSOR style fields, we don't need to calculate the pixel index
  - When we have rectangular pixels, isWithinMatrix(local_pos) can be much simpler than calculating pixel index first

Super-Charged pow() !1012

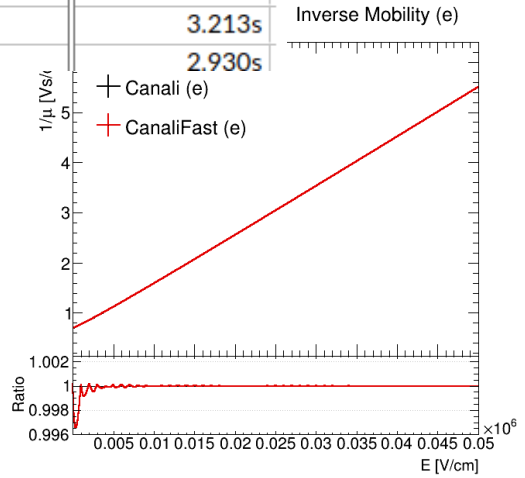
- *pow()* calls in mobility calculations are the hottest snippets in the execution for high-precision propagations
  - β is a constant after all …

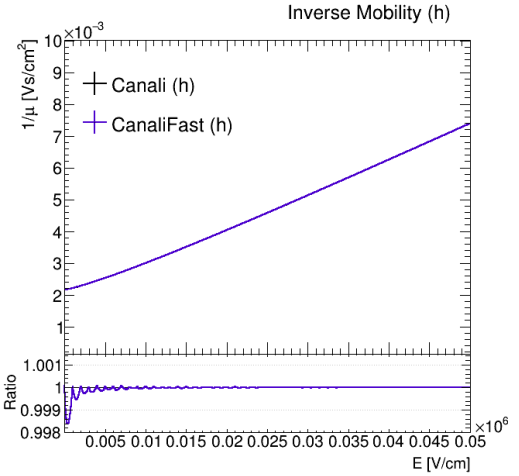
$$\mu(E) = \frac{v_m}{E_c} \frac{1}{(1 + (E/E_c)^{\beta})^{1/\beta}}$$

Function / Call Stack	CPU Time ▼
__pow	22.995s
allpix::DetectorField<ROOT::Math::DisplacementVector3D<ROOT::Math::Cartes	3.888s
std::mersenne_twister_engine<unsigned long, (unsigned long)64, (unsigned long)	3.347s
operator()	3.213s
llround	2.930s

```
mobility_model = canali_fast
```

- New implementation pre-calculates lookup table of pow(x, β) during initialisation
  - ➔ > 30% speed up possible
  - ➔ < 0.2% deviation from calculation at runtime





… And More …

OS Support

- Linux (!1089):
  - CentOS7 will be removed (EoL in 06/24)
  - LXPLUS moved to RHEL9 already
    - ➔ We drop CentOS9 and move to AlmaLinux 9 (EoL in 2032)
- MacOS (!1098 & !1099):
  - Mac support has been dropped
    - No further CI on Mac runners
    - No deployment via *CVMFS*
  - This doesn’t mean that Allpix Squared will not run on Mac anymore …
    - We will be happy to receive feedback and/or merge requests to maintain the usability of Allpix Squared on MacOS

Improvements …

- Register an exception handler already during geometry construction to catch any Geant4 exceptions raised there (!1029)
- *CSADigitizer*: addition and renaming of parameters – defaults backwards compatible (!1051)
- List unused keywords now also for geometry and model file – up to now only possible for main configuration file (!1075)

```
|12:12:57.876| (WARNING) Section [dummy_section1] is not valid in sensor geometry definition.
|12:12:57.876| (WARNING) Unused configuration keys in global section of sensor geometry definition:
                         dummy_parameter1
                         dummy_parameter2
```

- *MCParticle*: register and store particle energy at sensor entry and exit point (GH #45, see talk by Sam on Friday)
- *Masetti(-Canali)* mobility models differ depending on the n-dopant (!1016)
  - The dopant can now be selected via the configuration file (only used in Masetti models)

```
mobility_model =  masetti
dopant_n =        arsenic
```

… and Bugfixes

- Local and global times of *PixelCharge* objects are now non-zero when using *PulseTransfer* (!1027)
- Fixed implant collision detection in case of rectangular implants with offsets (!1040)
- *DepositionLaser*: fix beam waist definition (!1039)
- …

Summary

Summary

- Release of **v3.1** after one year of development
- **Major changes**:
  - Breaking changes to propagation algorithm
  - New beam types & deposition scanning techniques
  - Strong performance improvements
  - Drop macOS support
- Several projects are under development – see details in talk by Simon (Friday)

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