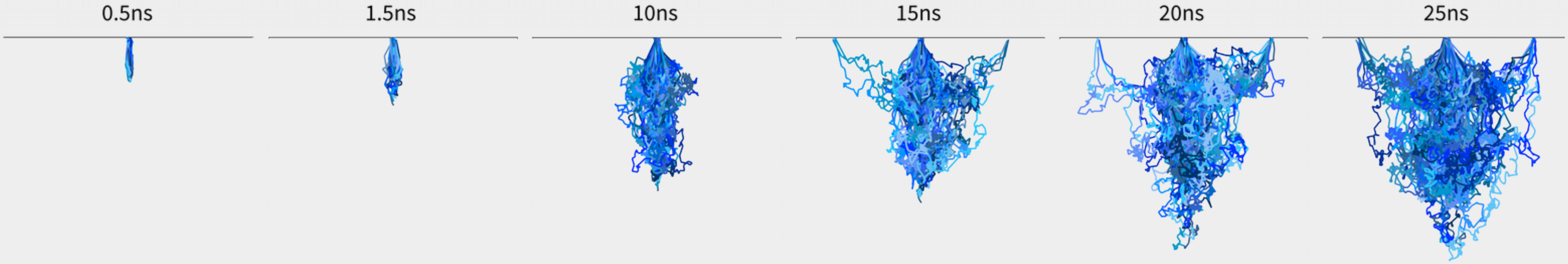
cern.ch/allpix-squared



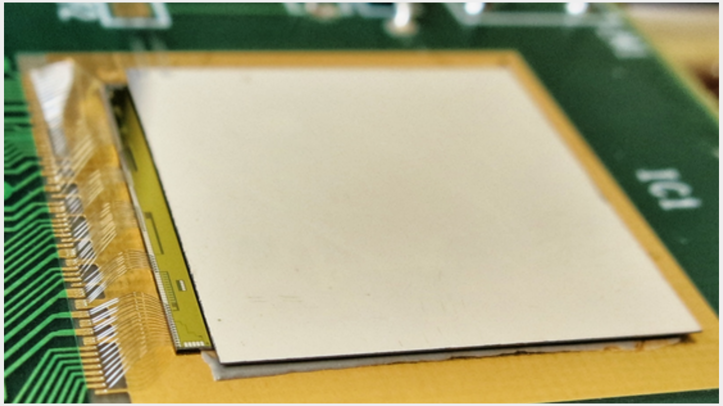
The Importance of Insight

Monte Carlo Simulations in Silicon Pixel Detector Development

Simon Spannagel, CERN
DESY Instrumentation Seminar
9 August 2019

Silicon Pixel Detectors in High Energy Physics

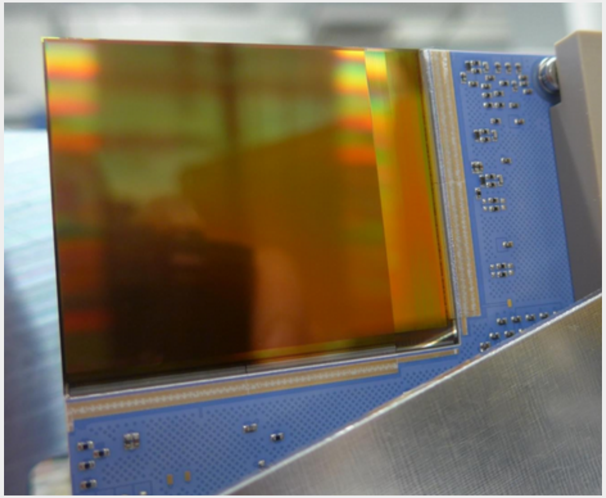
- Crucial in today's experiments: primary/secondary vertex resolution, pile-up reduction
- Demands on detectors are high:
  - Maximum resolution @ minimum (scattering-) mass
  - Very high granularity for high particle rates, fast readout, minimal dead time
  - "Smart" detectors (zero suppression, clustering, on-chip processing)



100 µm Timepix with 100 µm Sensor

- Initially, HEP was innovation driver
- Understanding technologies, behavior with radiation etc. known technologies
- Lately: catching up to more recent (imaging!) technologies used in industry – interesting features, but complex designs

Silicon Pixel Detectors in Photon Science

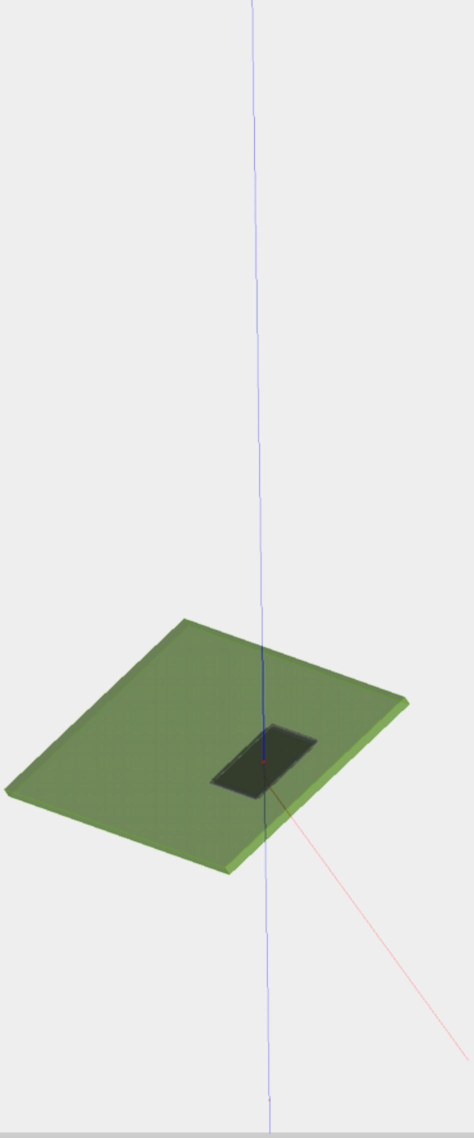

Percival

- Demands are different – but equally challenging
  - Large area imaging sensors
  - High frame rate at very low noise
  - Single photon sensitivity plus large dynamic range
- High-Z materials of interest
  - Much smaller absorption length for 1-100 keV photons
  - Not as many models for sensor response around as for silicon

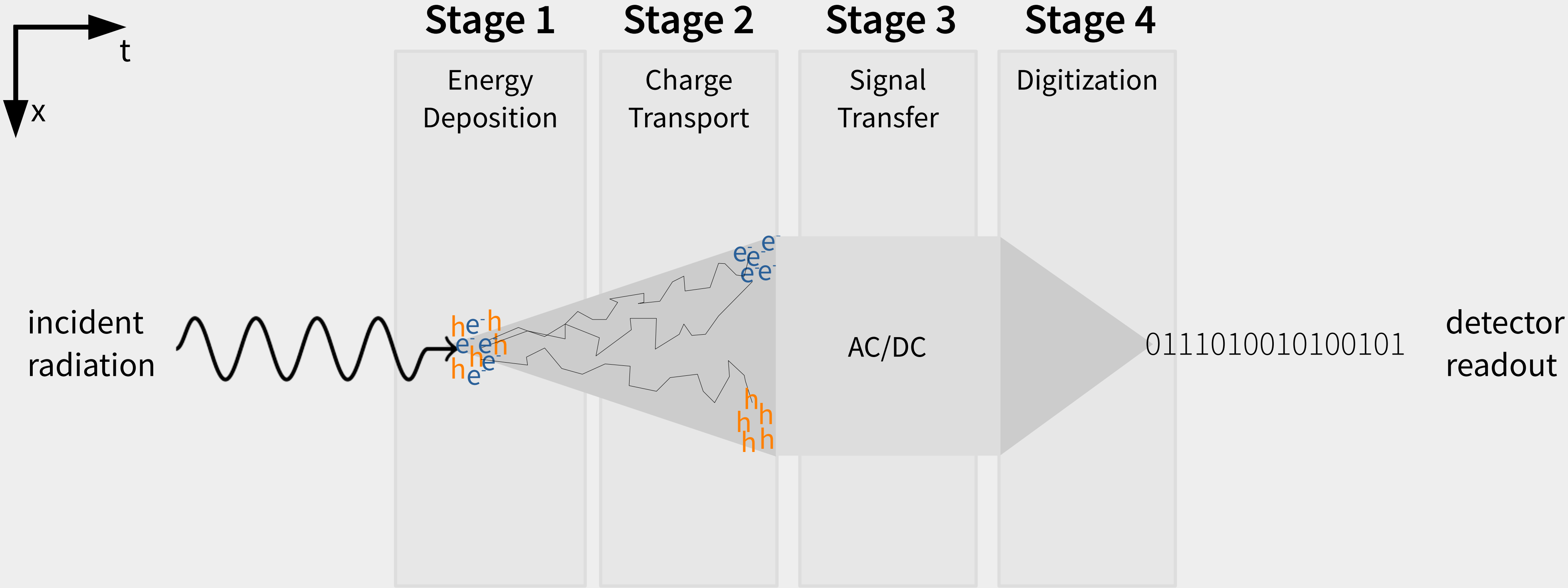
- Overlap with HEP in sensor technology used, difference e.g. in material budget
- Similar challenges in designing detectors in new deep sub-micron CMOS

Introduction

Particle Detection with Silicon Detectors

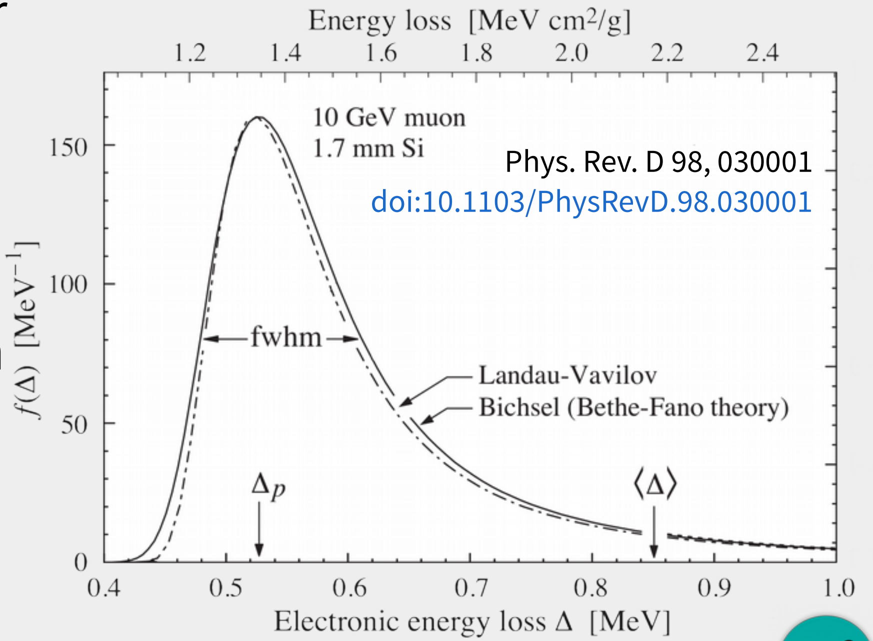


Recap: Particle Detection with Silicon Detectors



Stage 1 – Energy Deposition

- (heavy) charged particles:
  Mean energy loss described by **Bethe Bloch** formula
- Strong fluctuations of energy loss: **Landau-Vavilov** distribution / **Bichsel** model
  - Varying number interactions, energy transfer
  - Secondary particles (e.g. delta rays)
  - Most probable value < Mean
- Photons:
  Photo effect, Compton effect, pair production
- Creation of e/h pairs: 3.64 eV / pair
  Fluctuations: **Fano** Factor $\sigma_{e/h}=\sqrt{N_{e/h}}\sqrt{F}$



Phys. Rev. D 98, 030001
doi:10.1103/PhysRevD.98.030001

Stage 2 – Signal Formation

- Si sensor operated as diode in reverse bias → depleted volume
- Signal formed by motion of e/h pairs in electric field
- Contribution to motion:
  - **Diffusion** – Temperature-driven random motion, mean free path ~ 0.1 µm, mean 0
  - **Drift** – Directed motion, depending on electric field and charge carrier mobility, different parametrizations for mobility available, depending on temperature, silicon, ...
- Motion stops, when...
  - Charge carriers reach readout electrode (conductor)
  - Charge carriers recombine/get trapped (depends on purity, doping, lattice defects, …)
- When carriers reach electrodes, total induced charge is equivalent to collected charge

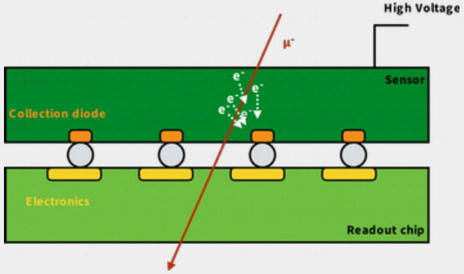
Stage 3 – Signal Transfer

- Coupling between sensor & front-end can be
    - DC: bump bonds (hybrid pixel), direct (monolithic pixel)
    - AC: glue layers (hybrid pixel), SiO_2 (strip detectors)

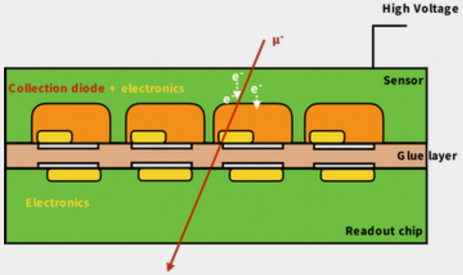
Stage 4 – Digitization

- Signal is amplified, shaped, zero-suppression (discriminator)
- Digitization of the signal via
    - Full ADC
    - Time-over -threshold
    - Threshold crossing (binary hit information)
- Buffering, encoding, data transmission…

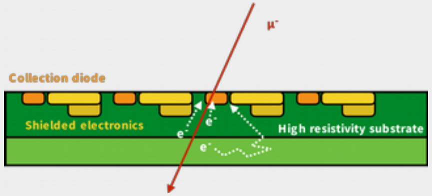
bumped hybrid



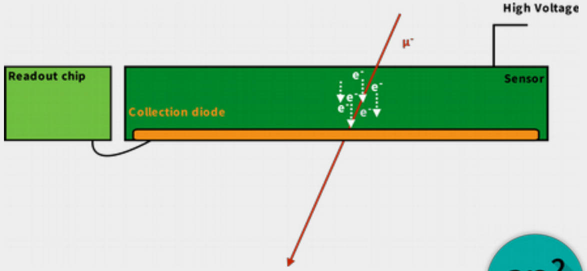
glued hybrid

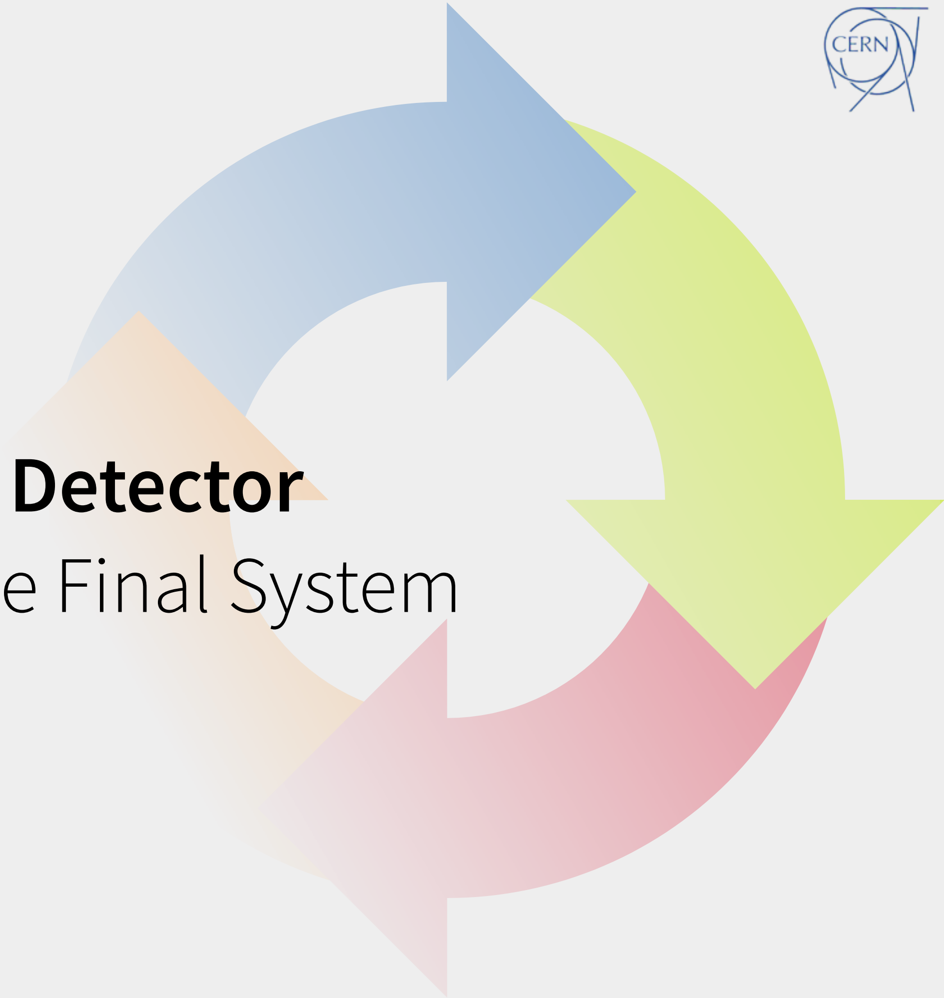


monolithic



strip

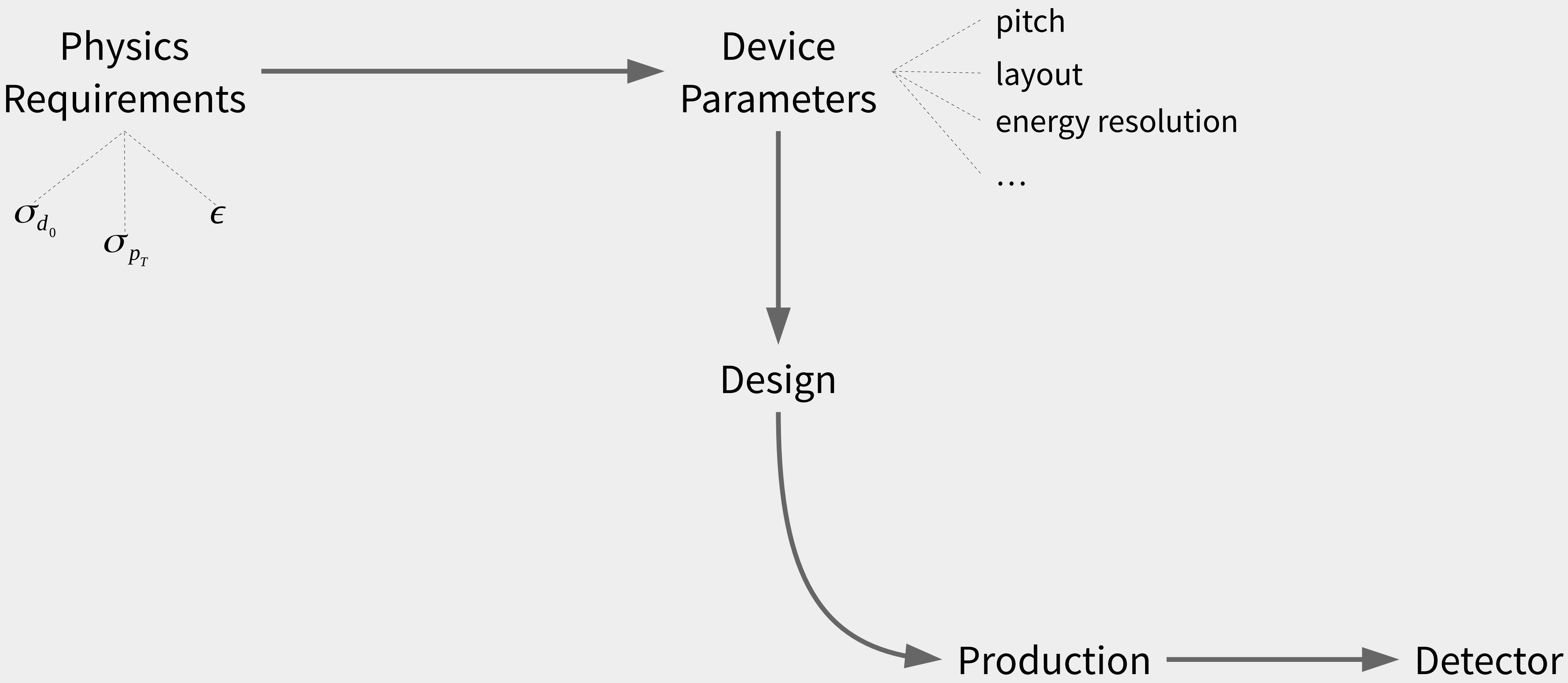




Development Cycle of a Silicon Detector

From Physics Requirements to the Final System

Development Cycle of a Silicon Detector



Physics Requirements

σ_{d_0} σ_{p_T} ϵ

Device Parameters

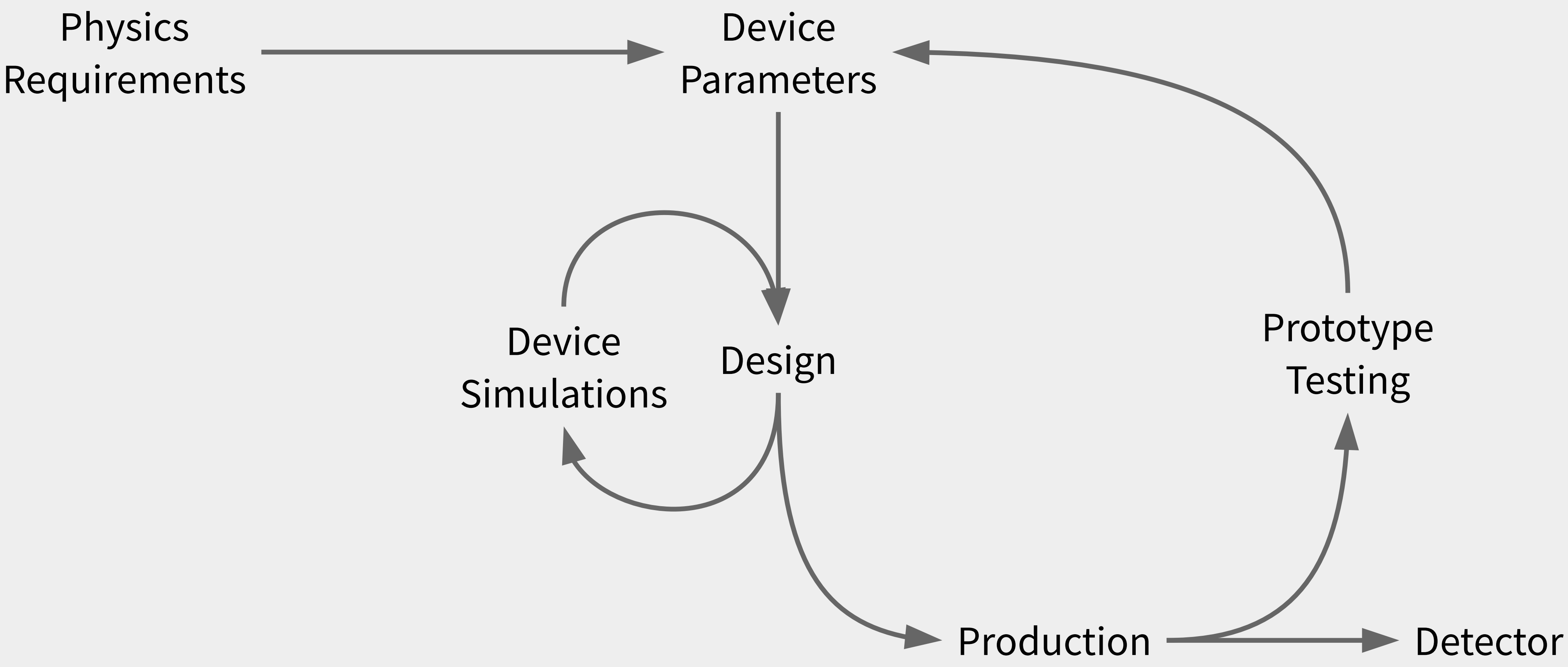
- pitch
- layout
- energy resolution
- …

Design

Production

Detector

Development Cycle of a Silicon Detector



Physics Requirements

Device Parameters

Device Simulations

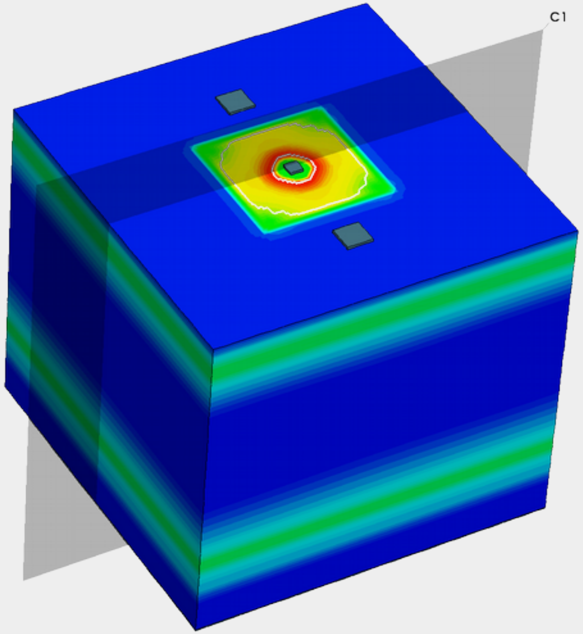
Design

Prototype Testing

Production

Detector

TCAD Sensor Simulations

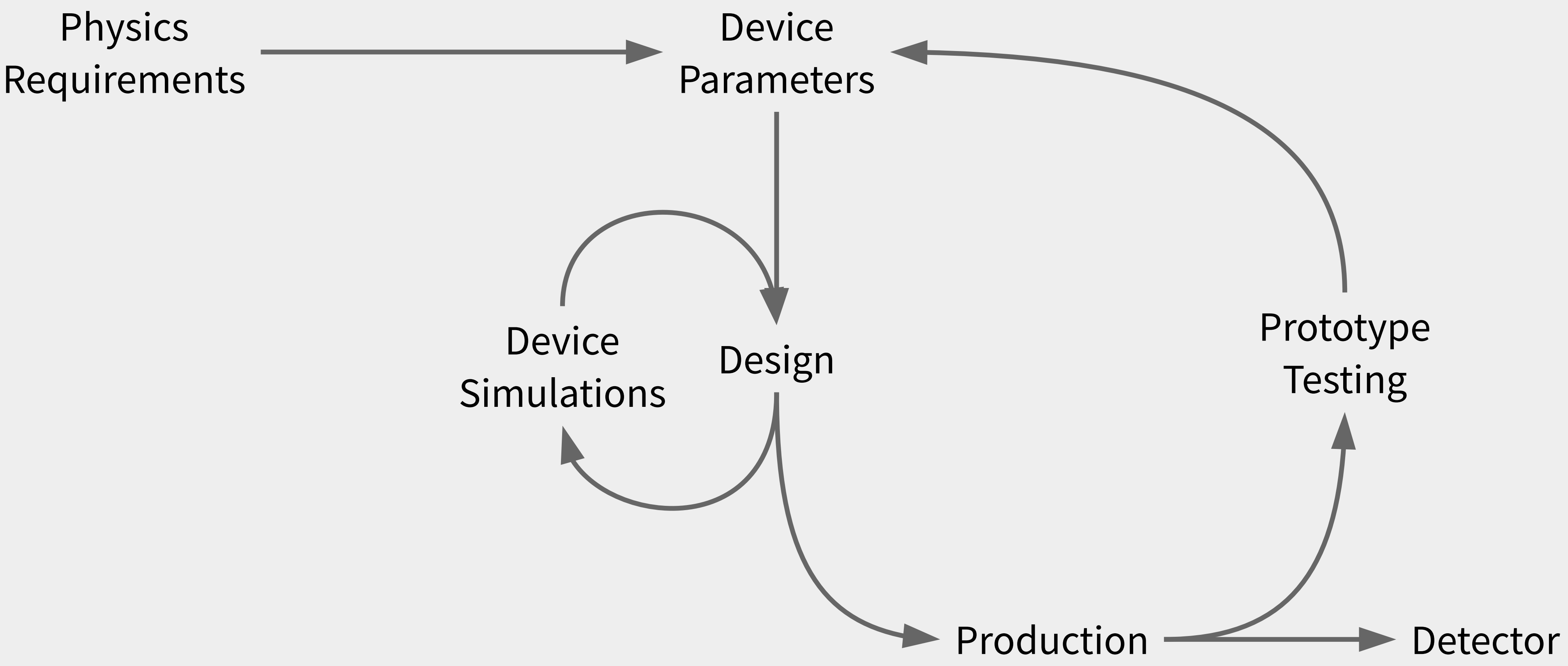


- *Technology Computer Aided Design*
    - Simulate electrical properties of semiconductor by numerically solving field equations on mesh
- Requires knowledge of the production process (doping concentrations, implants)
- Provide detailed information on
    - Field configuration of the device
    - Derived parameters: depletion voltage, break down voltage
- Also allows to perform time-resolved transient simulations: current pulses
    - Very time consuming, especially in 3D
    - Periodic boundary conditions might allow to reduce complexity

Front-End Circuit Simulation

- SPICE – *Simulation Program with Integrated Circuit Emphasis*
  - Simulate response of circuit to external stimuli
  - Many commercial derivatives, usually come with EDA software
- Based on IC design, either schematics or on netlist level
- Provides detailed information on
  - Response of front-end amplifier
  - Digitization process
- Works on individual input pulses
  - Time-consuming
  - Not really feasible to repeat for large number of input pulses

Development Cycle of a Silicon Detector



Physics Requirements

Device Parameters

Device Simulations

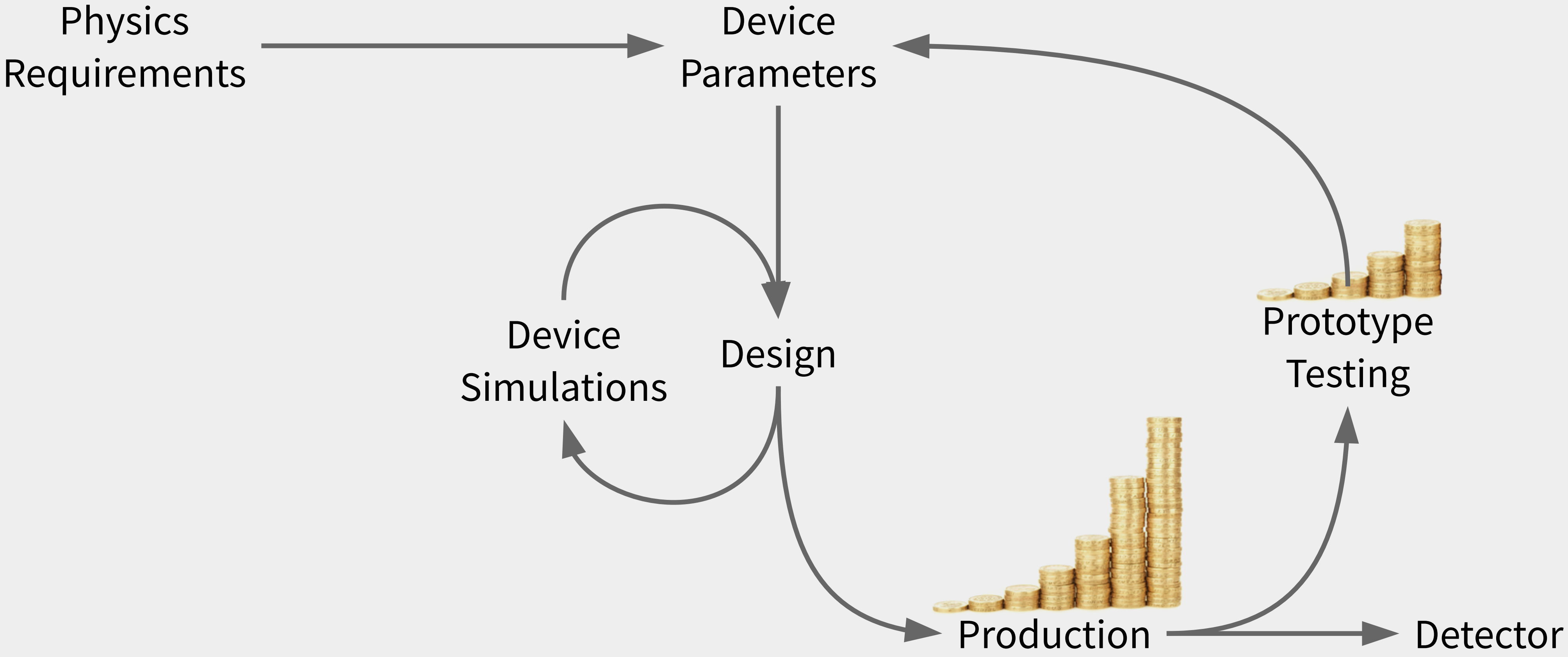
Design

Prototype Testing

Production

Detector

Development Cycle of a Silicon Detector



Physics Requirements

Device Parameters

Device Simulations

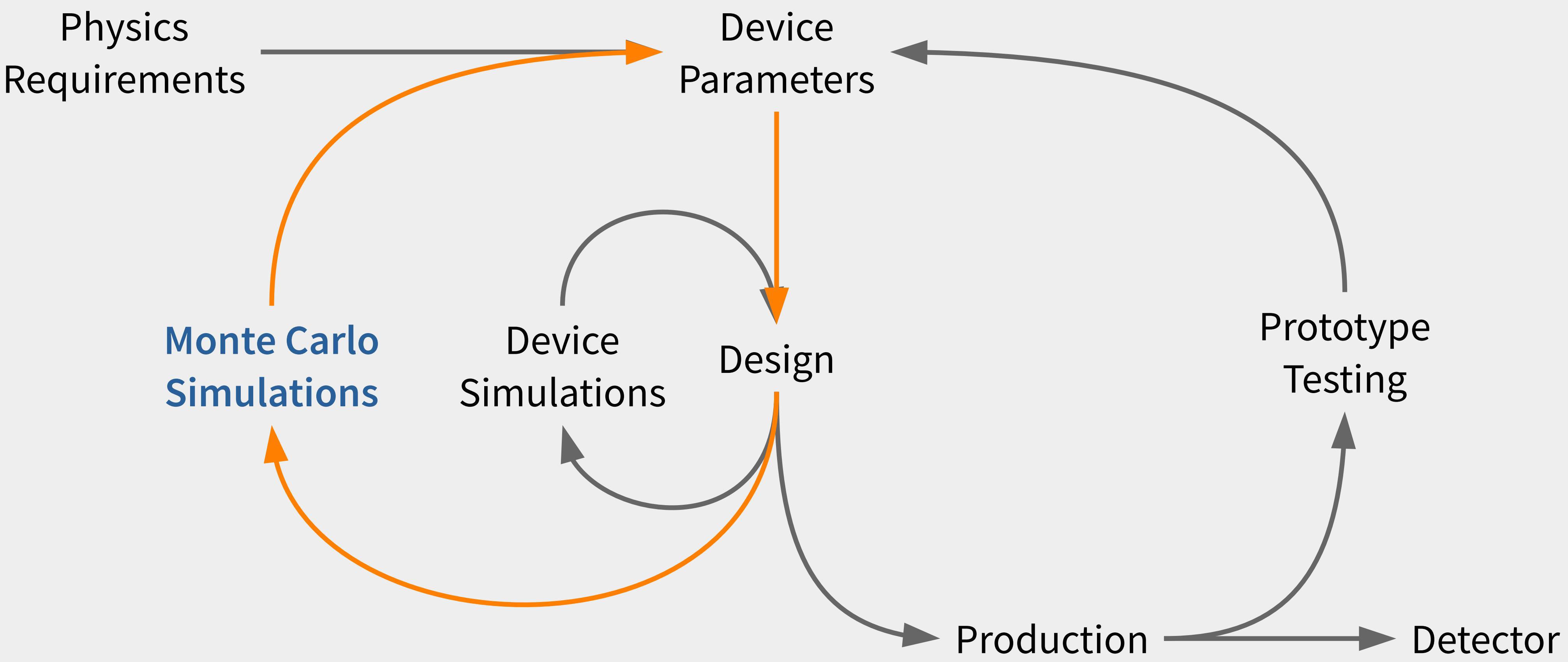
Design

Prototype Testing

Production

Detector

Development Cycle of a Silicon Detector



Physics Requirements

Device Parameters

Monte Carlo Simulations

Device Simulations

Design

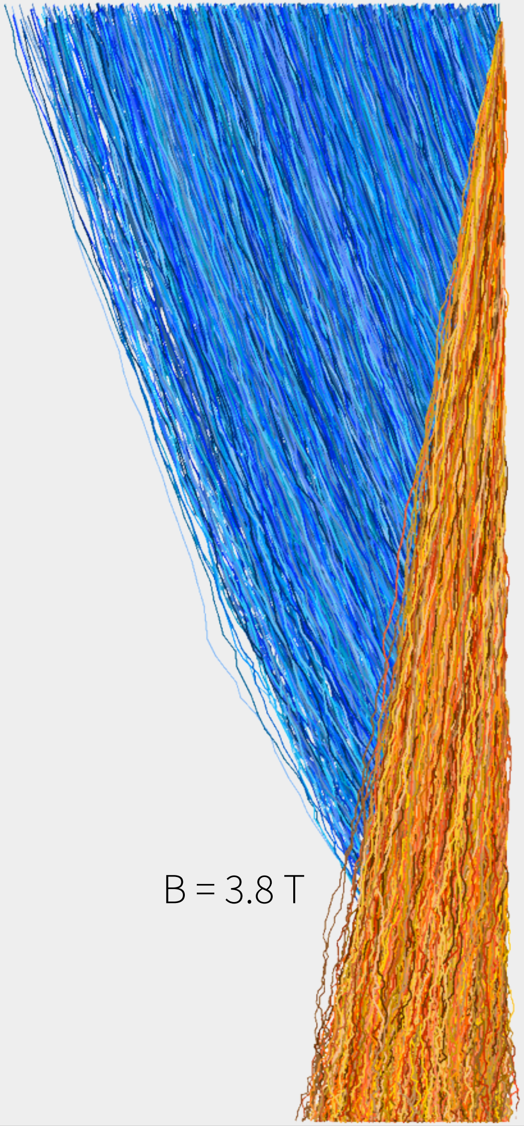
Prototype Testing

Production

Detector

Monte Carlo Simulations

Access to Performance Parameters



Monte Carlo Simulations

- Simulate full chain: energy deposition → readout
- Include stochastic effects, fluctuations, secondaries
- Requires **simplifications**:
  - No self-interaction, static electric field, …
  - Empirical models for different stages
- Allows to derive **performance parameters**
  - Position resolution, timing, efficiency
  - Combine with results from device simulations to increase accuracy
- Monte Carlo Simulation Codes:
  AllPix, PixelAV, KdetSim, Garfield++, (unpublished codes), …, **Allpix Squared**

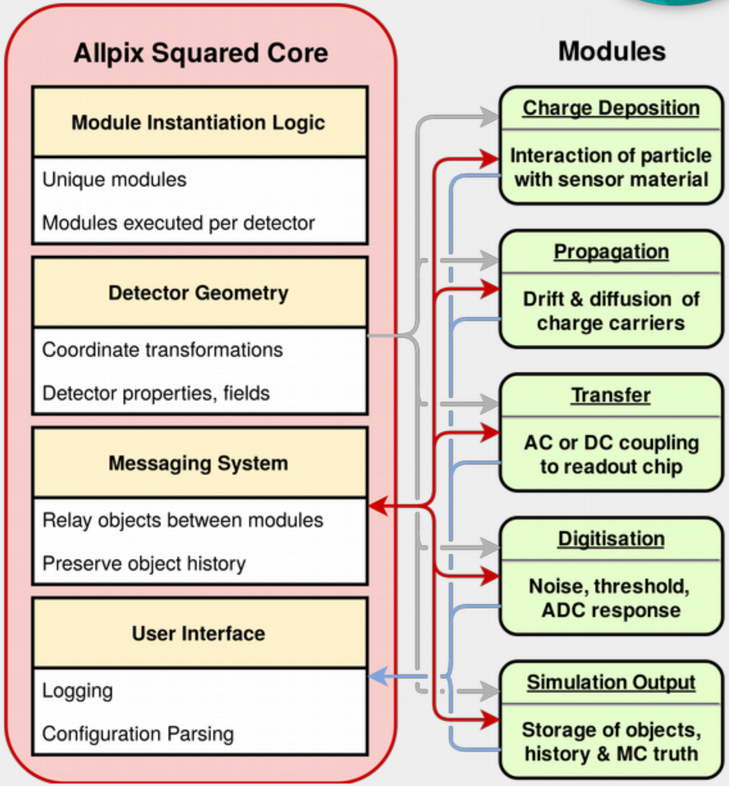
The Allpix² Framework

- Flexible MC simulation software, that

  ...allows to **test different** simulation **models for** signal formation

  ...implements parametrized detector models

  ...facilitates usage of **precise electric fields**
- Focus on usability
  - Separate infrastructure from physics
  - Easy setup & configuration
  - Provide documentation (150p. user manual)
- Developed within **CLICdp collaboration**



Allpix Squared Core

Module Instantiation Logic

Unique modules

Modules executed per detector

Detector Geometry

Coordinate transformations

Detector properties, fields

Messaging System

Relay objects between modules

Preserve object history

User Interface

Logging

Configuration Parsing

Modules

Charge Deposition

Interaction of particle with sensor material

Propagation

Drift & diffusion of charge carriers

Transfer

AC or DC coupling to readout chip

Digitisation

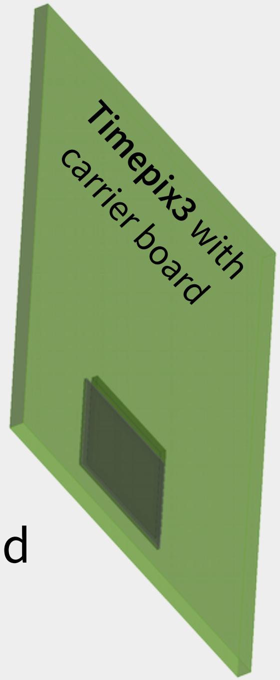
Noise, threshold, ADC response

Simulation Output

Storage of objects, history & MC truth

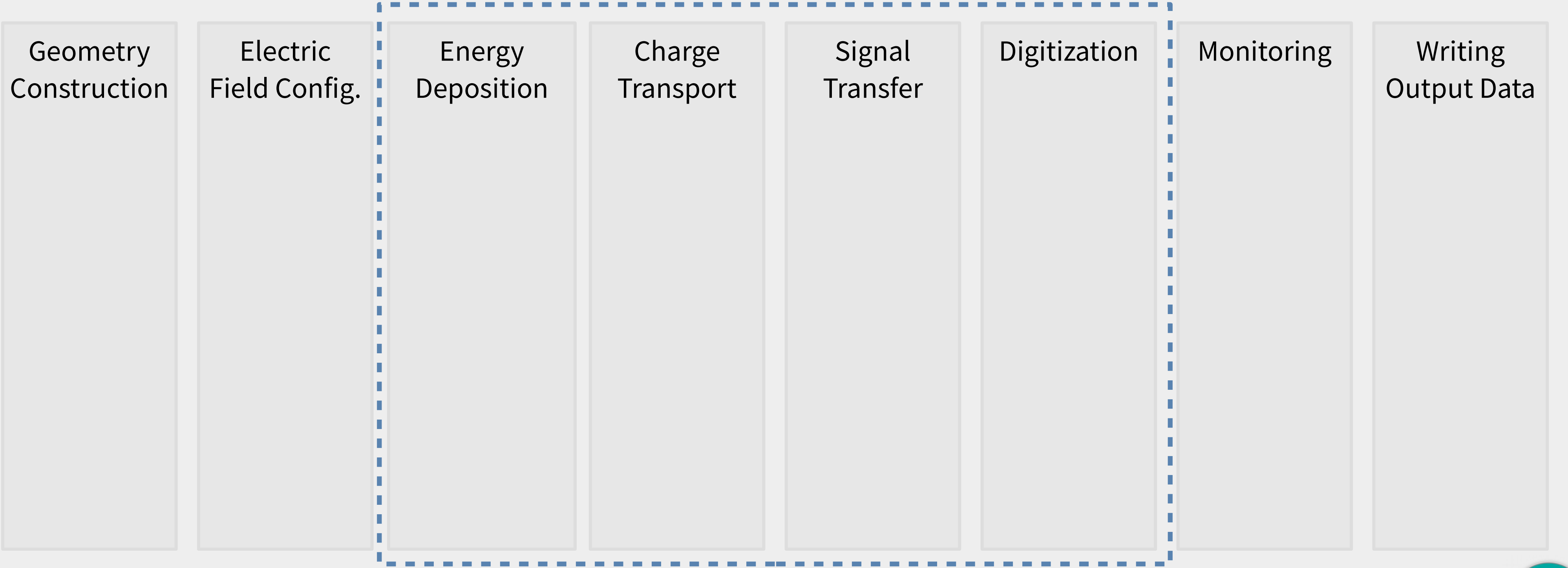
Configuration of the Simulation Chain

- Building simulation chain from individual modules
  - Configuration file with modules in order of execution
  - Support for physical units
- Every parameter documented in manual
- Geometry configuration
  - File with position/orientation of individual detectors
  - Model files define detector geometries
  - Different detector models pre-configured



```
[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]
```

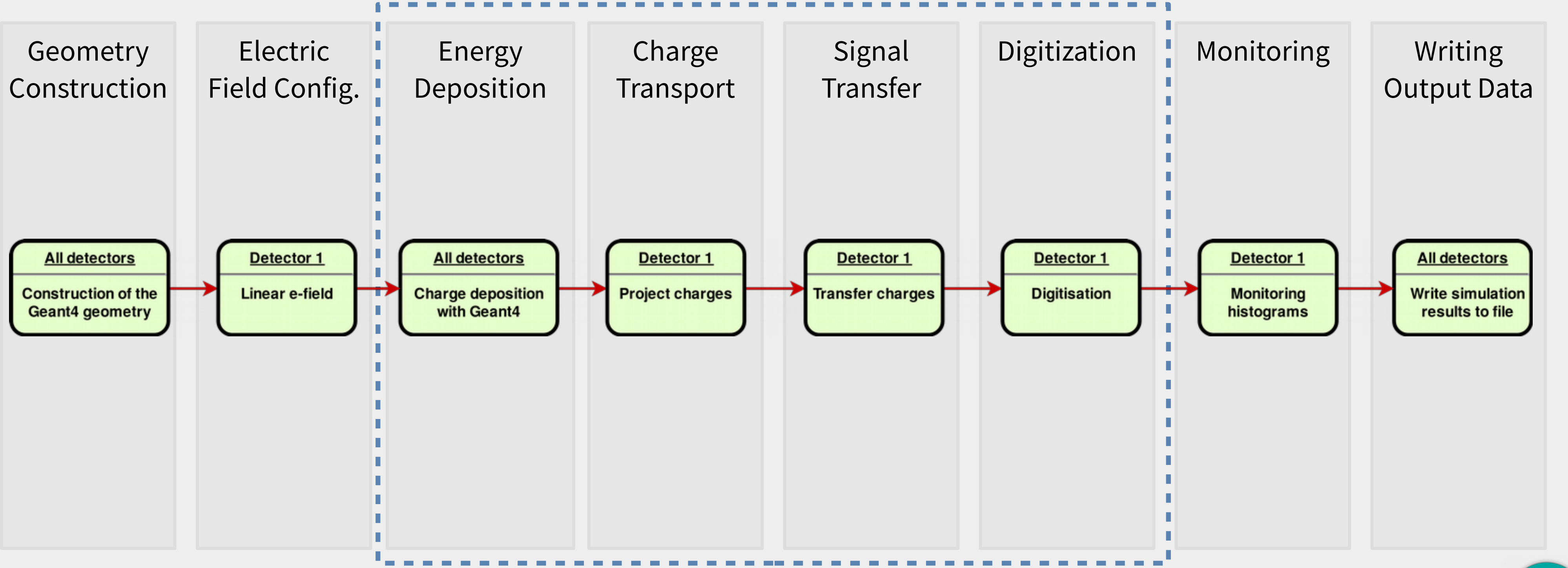
The Simulation Chain



- Geometry Construction
- Electric Field Config.
- Energy Deposition
- Charge Transport
- Signal Transfer
- Digitization
- Monitoring
- Writing Output Data

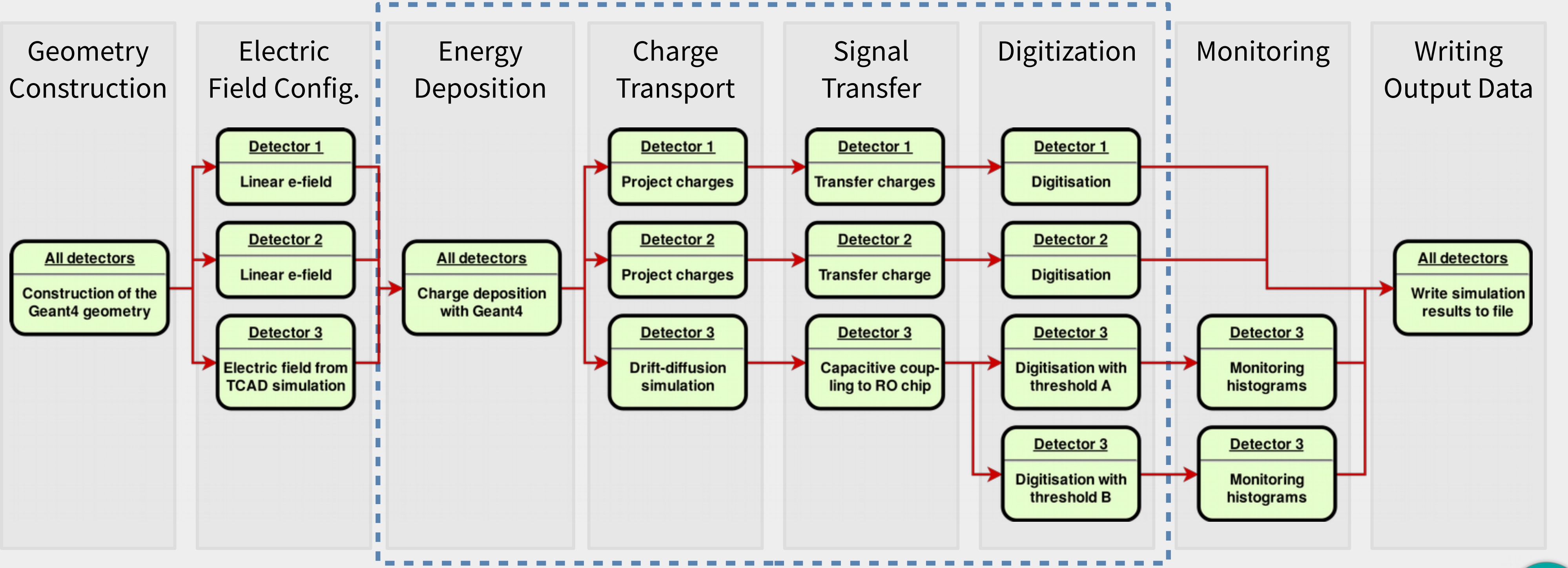
The Simulation Chain

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



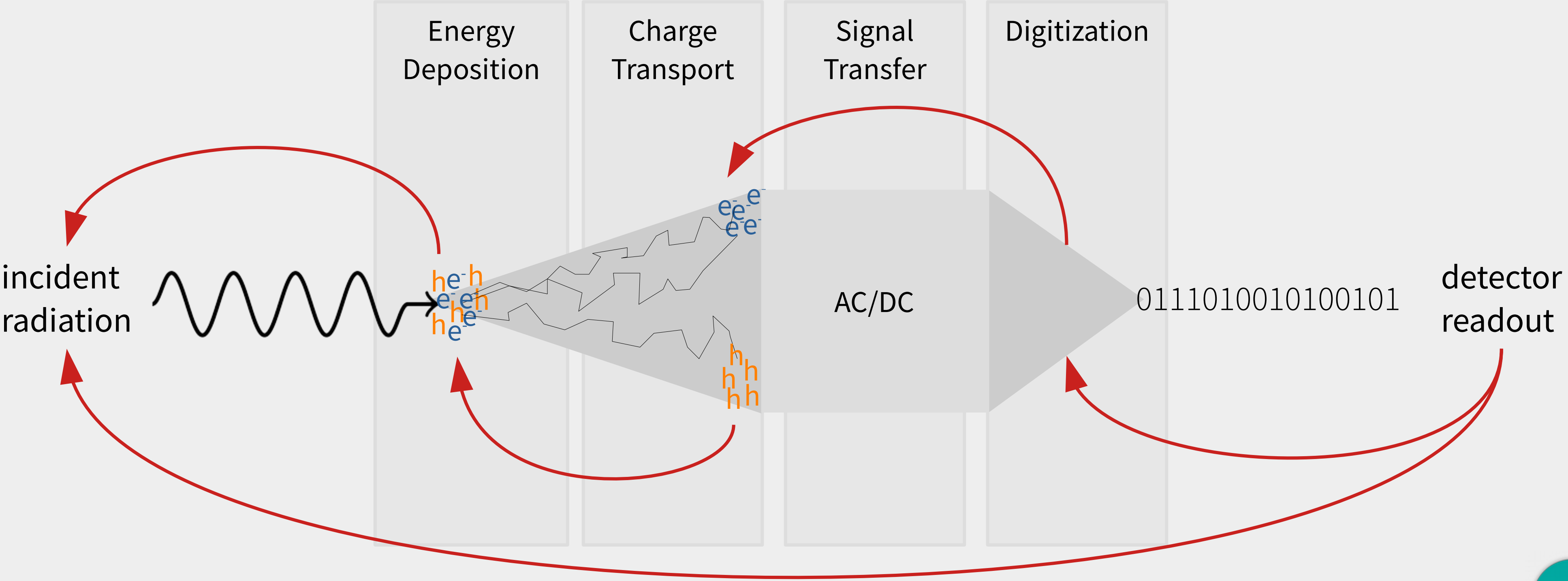
The Simulation Chain

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



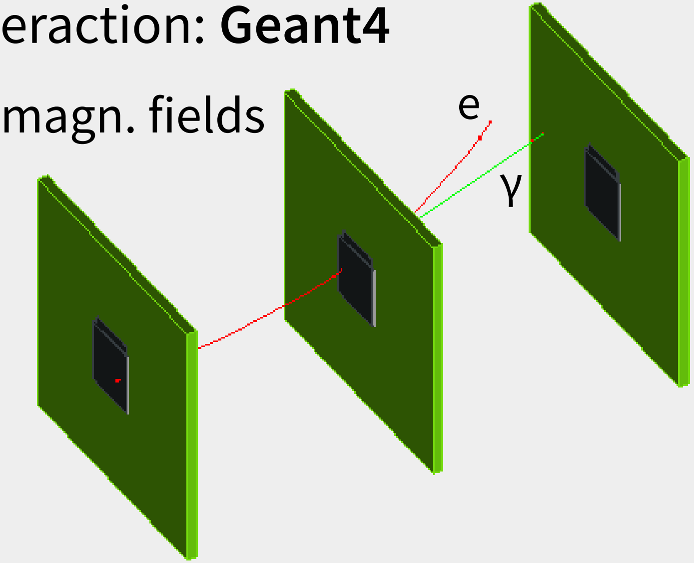
The Monte Carlo Truth

- Unlike in nature, in simulations we know everything
- Allpix^2 keeps history for all simulated objects – available for detailed analysis



Energy Deposition

- Using established software for simulating particle interaction: **Geant4**
  - Tracking of particles through entire setup, including magn. fields
  - Production and tracking of secondary particles
  - Provides MC truth information on all particles
  - Allows visualization of setup



- Possible alternatives:
  - Very simple model: Depositing charge at single point or along line
  - Custom code using energy loss spectra and lookup tables delta ray ranges
  - Custom code for simulation of laser measurements

Charge Transport

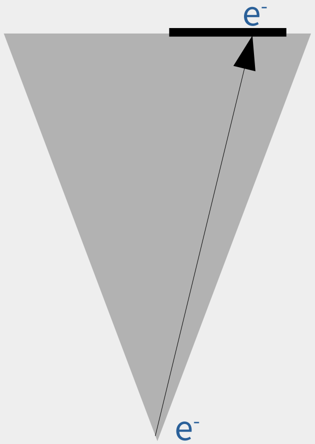
- Most crucial (and time consuming) component in simulation chain
- Various models with different complexity:
    - O(1) – Projecting Charge Carriers
    - O(N) – Integration of Equations of Motion
    - O(2xNxM) – Induced Signal at Electrodes
- Multiple charge carriers from same energy deposit propagated together
    - Depending on initial statistics and required accuracy
    - Some models allow to ignore electrons or holes
- Computing time given per group of charge carriers

O(1) – Projecting Charge Carriers

- With linear electric field, calculate approximate total drift time via analytical approximation of mobility integral
- For each (group of) charge carrier,
  - Calculate total drift time
  - Calculate total diffusion offset for this time
  - Put charge carrier on sensor surface, with offset drawn from Gaussian distribution of width σ_x
- Very fast simulation, few calculations
- Only works for linear electric field approximations (reasonable for many thick planar sensors) and without magnetic field

$$t = \int \frac{1}{v} ds \approx \frac{1}{\mu_0} \left[\frac{\ln(E(s))}{k} + \frac{s}{E_c} \right]_a^b$$

$$E(s) = ks + E_0$$

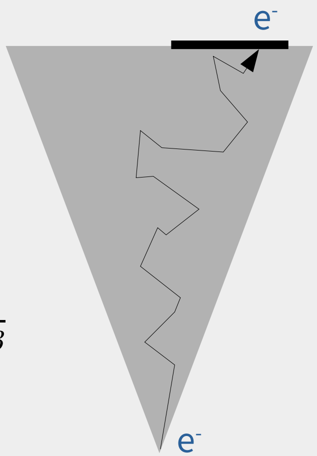


O(N) – Integration of Equations of Motion

- Successive integration of charge carrier motion
- Take each (group of) charge carrier
  - Calculate mobility μ from local electric (and magnetic) field (using Jacoboni/Canali parametrization)
  - Calculate velocity
  - Make step, add diffusion offset from Gaussian distribution
  - Repeat N times until sensor surface is reached
- Using 5th order Runge-Kutta-Fehlberg method
  - Adaptive step size according to position uncertainty
  - Method allows description of drift in complex field configurations

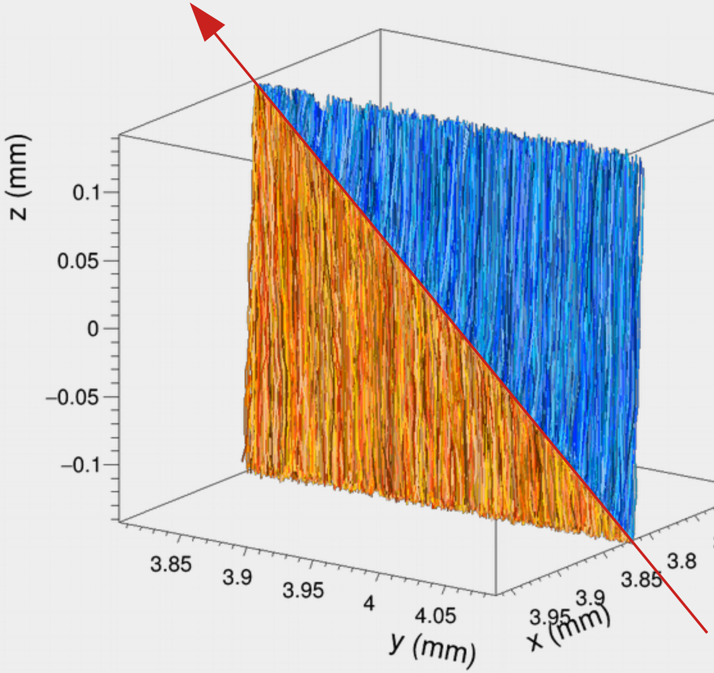
$$\mu=\frac{v_m}{E_c}\frac{1}{\left(1+\left(E/E_c\right)^{\beta}\right)^{1/\beta}}$$

$$\sigma_x=\sqrt{\frac{2k_bT}{e}\mu t}$$

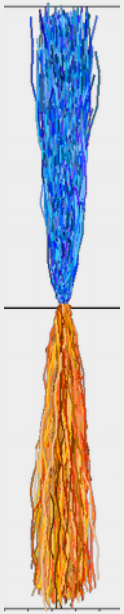


Drift Path Visualizations

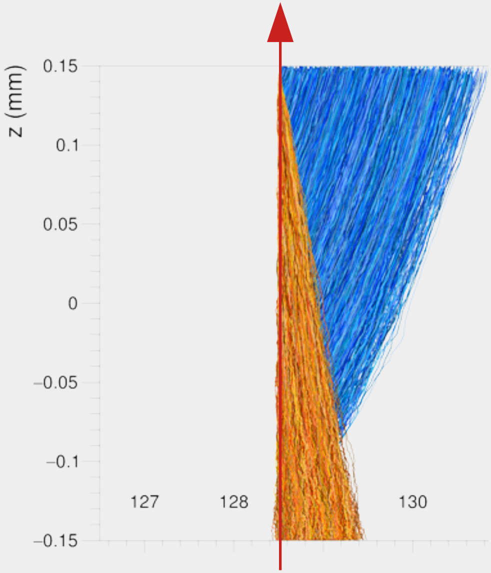
Recording individual steps of the RKF integration to produce visualizations



particle at 45° angle
drift paths of electrons & holes

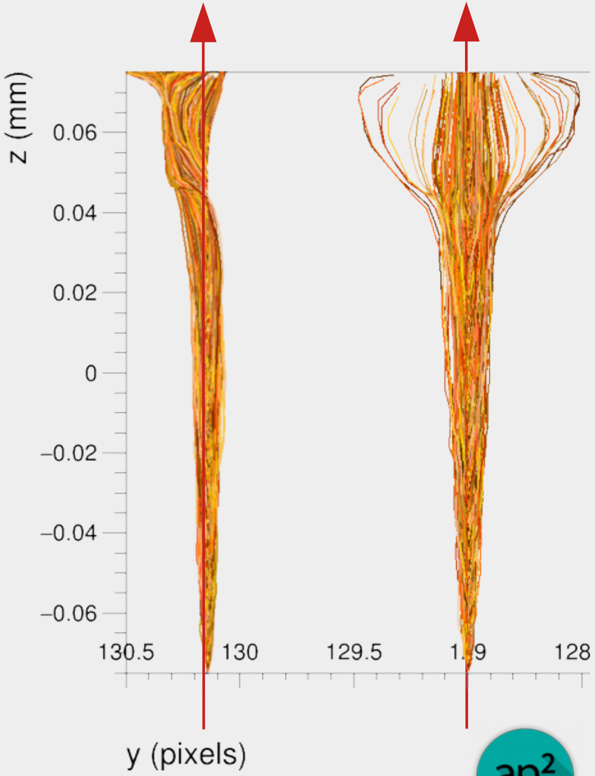


projection along trajectory



drift in magnetic field:
effect from Lorentz force

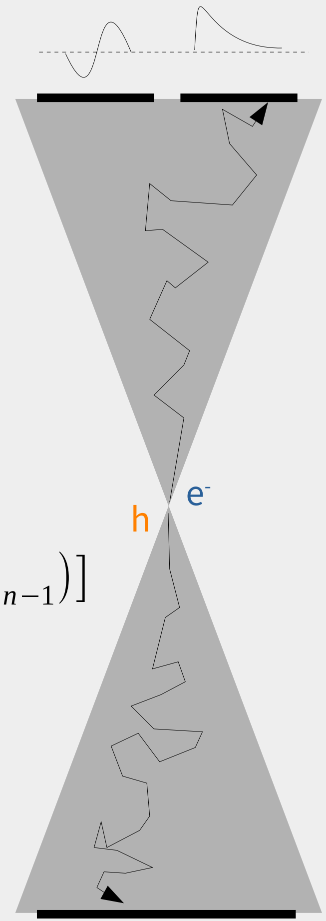
drift in non-trivial field:
ELAD sensor (holes only)



O(2xNxM) – Induced Signal at Electrodes

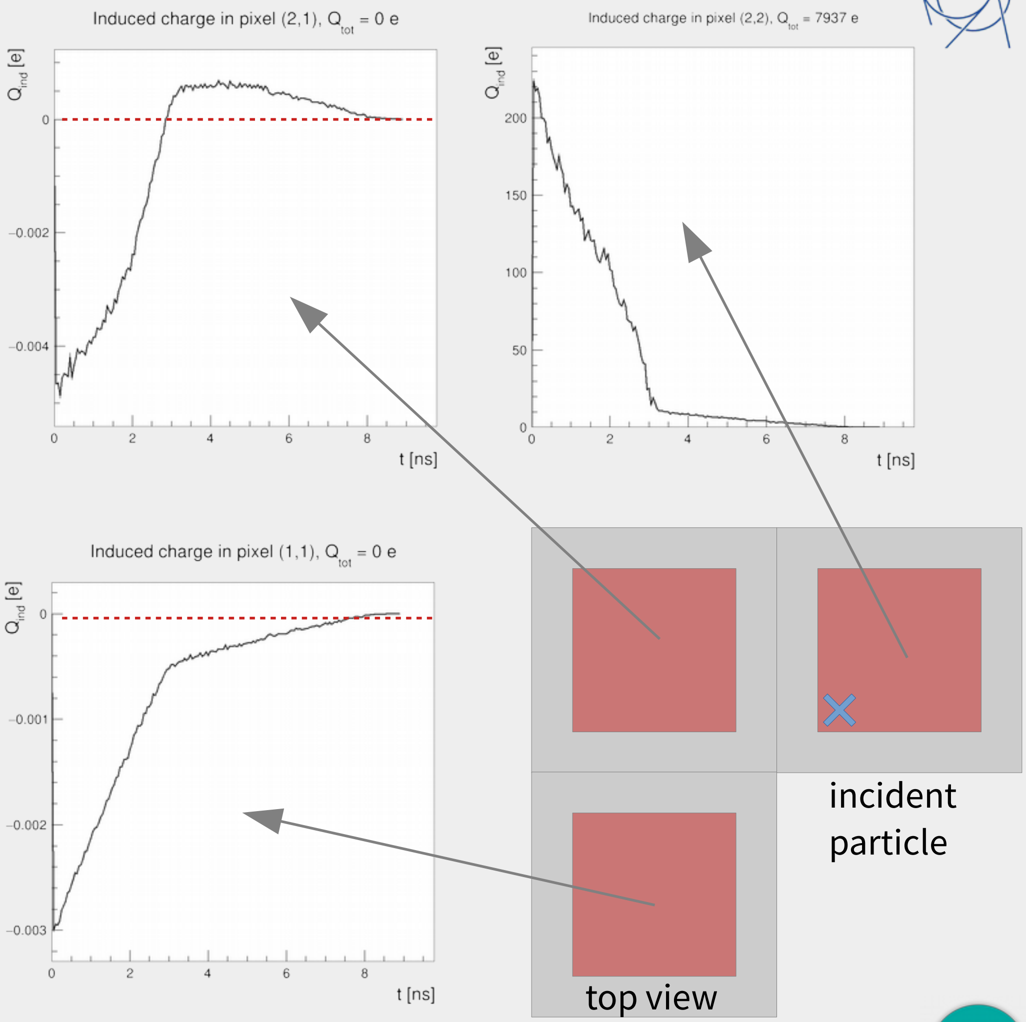
- Successive integration of motion, calculating induced charge per step
- Take each (group of) charge carrier
  - Calculate mobility & velocity from local fields
  - Make step, add diffusion offset from Gaussian distribution
  - Get induced charge from weighting potential difference for M neighbors
  - Repeat N times until sensor surface is reached
- Allows time-resolved simulation
  - Requires weighting potential, might not be trivial to obtain
- Time consuming:
  - Calculation for all neighboring electrodes for every step
  - Requires propagating both electrons and holes (x2)

$$Q_n^{ind.} = \int_{t_{n-1}}^{t_n} I_n^{ind.}\, dt = q\left[\phi(x_n) - \phi(x_{n-1})\right]$$



Current Pulses at Electrodes

- Example of transient simulation released in Allpix Squared 1.4
- Detector with
  - 300 µm x 300 µm pitch,
    200 µm x 200 µm electrodes,
    100 µm sensor thickness
  - MIP-equiv. Particle,
    80 e/h-pairs / µm
- Struck pixel sees total charge
- Neighbor pixels see tiny pulses,
  net charge is zero



Including Additional Effects

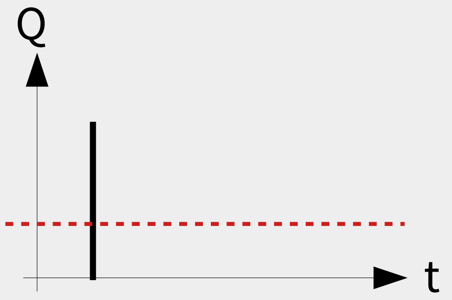
- Depending on simulation scenario, additional effects might be required
  - Slow sensors might expose effects from recombination
  - Irradiated sensors see strong effect from trapping
- Some can be added ad-hoc to propagation models:

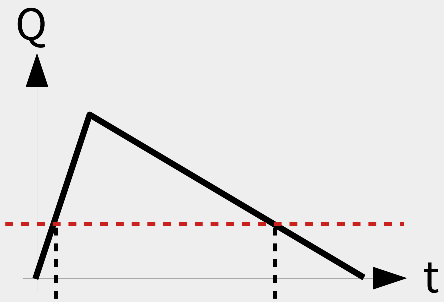
Trapping of carriers	(stop propagation for certain time)
Recombination	(stop propagation completely)
Multiplication	(create new charge carriers at strong electric fields)

- Other effects (shielding effects in electric field, charge carrier self-interaction) are more difficult to include, complexity might go beyond MC simulations

Digitization

- Methods depend on available information from charge transport:
- Simple front-end
  - Compare total charge against configured threshold
  - Add input noise, threshold dispersion, convert to ADC units
- Front-end with timing capabilities
  - Requires current pulse
  - Threshold crossings for time-of-arrival and time-over-threshold
- Full front-end simulation
  - Requires current pulse shape
  - Lookup tables for front-end response function, produced from device simulations



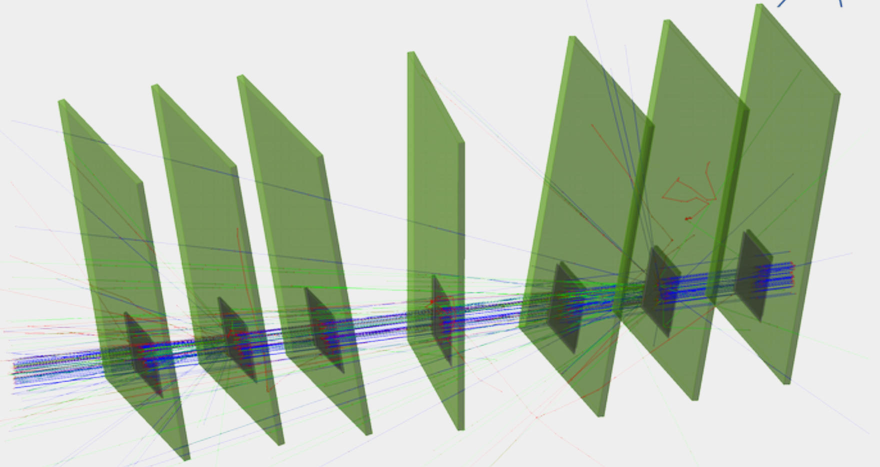


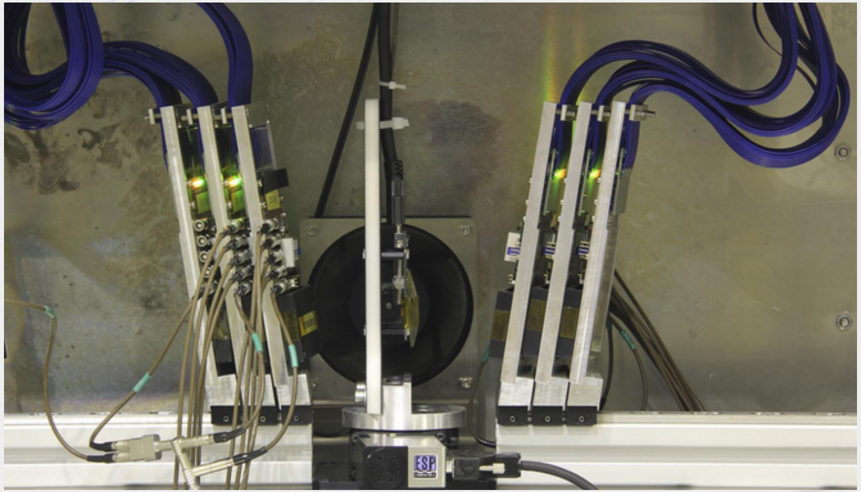
Examples

Planar, ELAD and CMOS Sensors

Simulation of Detector System

- Simulation of a beam telescope setup: CLICdp Timepix3 telescope @ SPS H6
  - Telescope: 6x Timepix3 w/ 300 µm sensors
  - DUT: 1x Timepix3 w/ 50 µm sensor
- Validation of reconstruction
- Different algorithms used:
  - Telescope: projection
    DUT: successive integration
- Linear electric field approximation



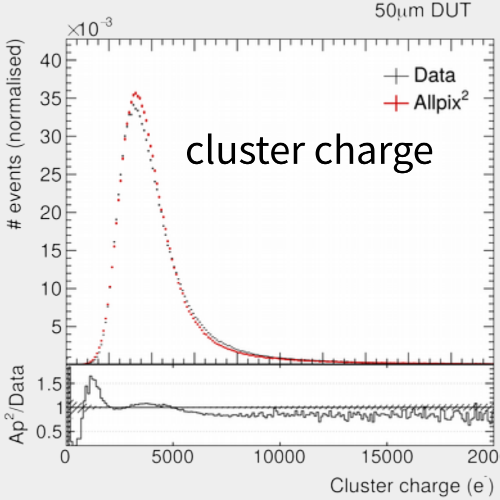


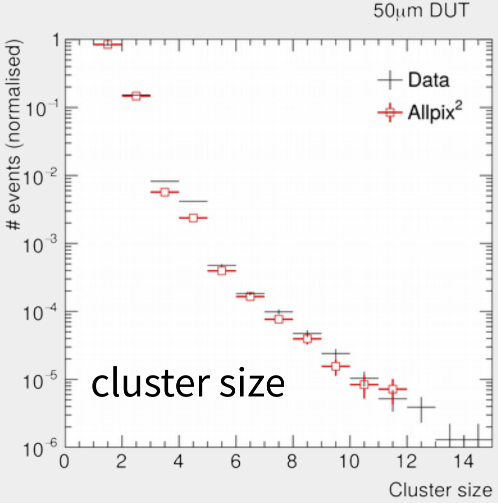
NIMA 901 (2018) 164 – 172

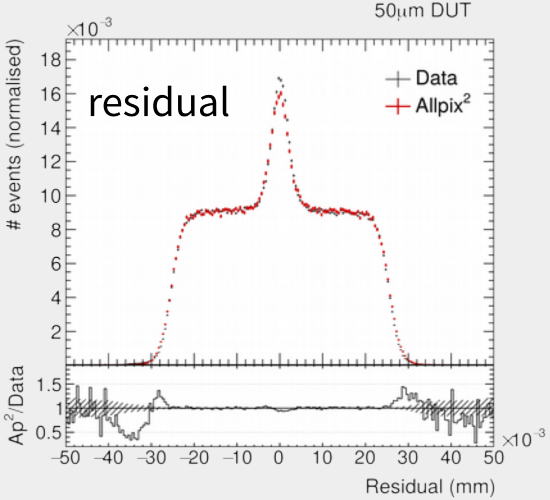
doi:10.1016/j.nima.2018.06.020

Simulation of Detector System

- Using same reconstruction algorithms as for data: clustering, η correction, tracking
- Very good agreement between data and simulation observed (total charge: **Geant4**; cluster size: both; residual shape: **Allpix^2**)

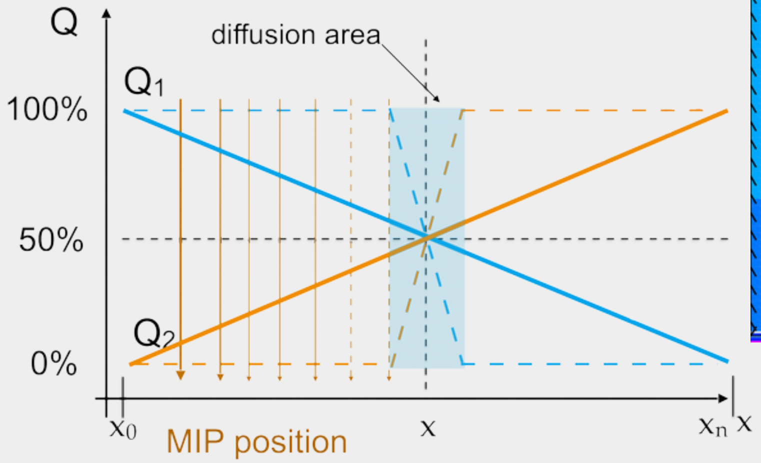


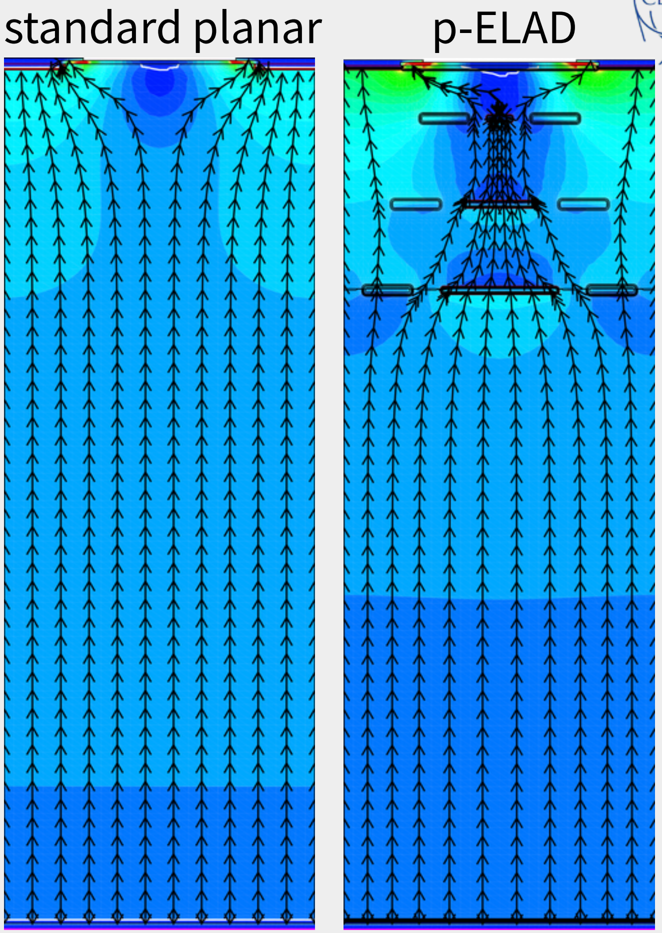




Enhanced Lateral Drift Sensors

- Resolution in **thin sensors** limited to pitch / √12
- **Enhance charge sharing** via electric field
  - Deep implants create lateral field
  - Spread of charges during drift, cluster size ~2
- Theoretical optimum: linear sharing
- No prototype yet: **use simulation to optimize sensor**

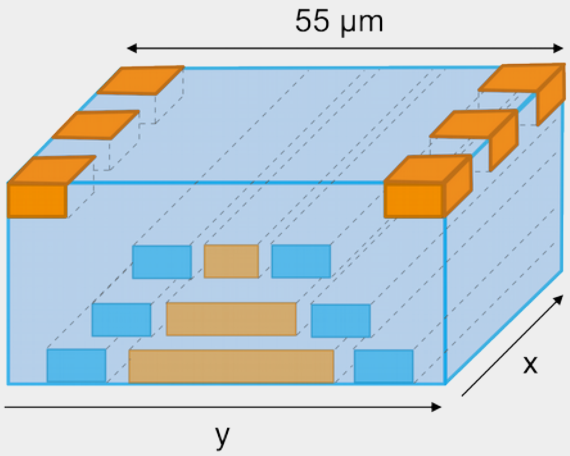


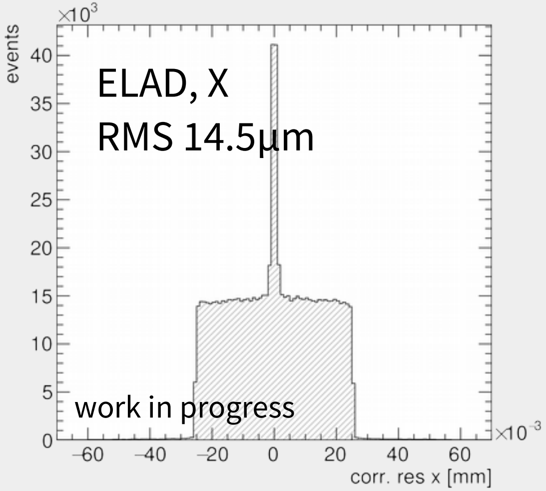


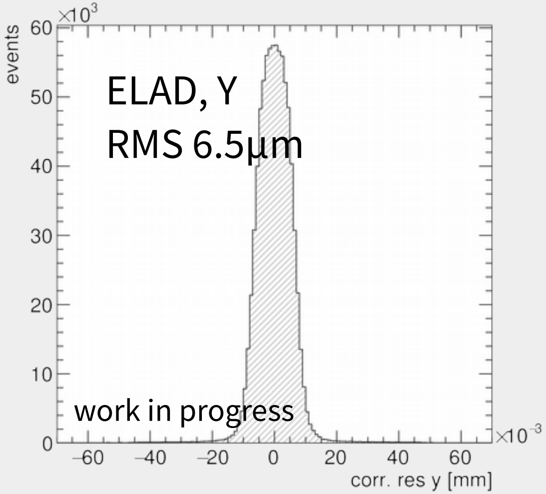
NIMA 831 (2016) 242 – 245
doi:10.1016/j.nima.2016.01.092

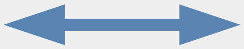
Enhanced Lateral Drift Sensors

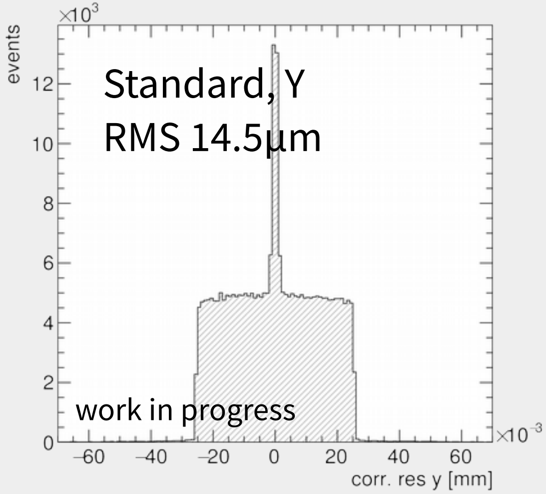
- MC Simulation with Timepix3 pitch: 55 µm
- Strip-like ELAD implants, expecting
  - X: Unaffected charge sharing along strip implants
  - Y: Stronger charge sharing across strip implants
- Using TCAD electric field & successive integration model





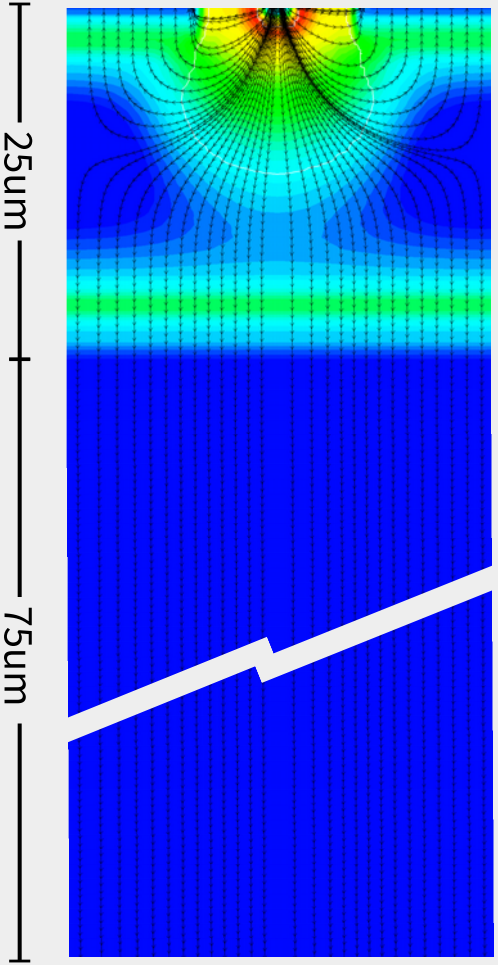






Monolithic CMOS in High-Resistivity Silicon

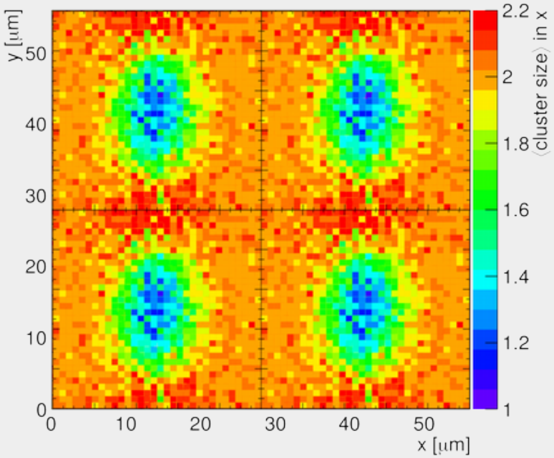
- ALICE Investigator chip, pixels with 28x28um pitch
  - Field in top 25um (high-resistivity) silicon
  - Undepleted in 75um silicon substrate
  - Measurements published: NIMA 927 (2019) 187-193 doi:10.1016/j.nima.2019.02.049
- Simulation compared to data from SPS, 120 GeV π
  - Simulating only detector under investigation
  - Using Monte Carlo truth information as reference
  - Smeared with telescope resolution obtained from data
- Electrostatic field obtained from TCAD simulations



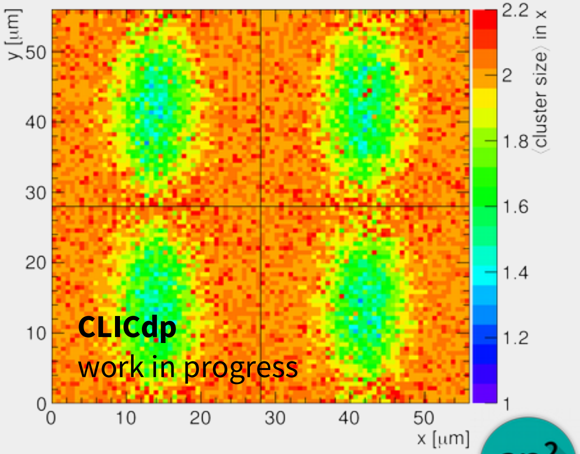
Monolithic CMOS in High-Resistivity Silicon

- High statistics of 3D Monte Carlo simulation:
  - Sampling of quantities within pixel cells
  - Here: cluster size in x
- Fully depleted planar sensors:
  expecting bands without y-dependence
- Cluster size exhibits correlation between x/y
  - Reason is field configuration & signal contributions from diffusion
  - Simulation with TCAD electric field reproduces correlation

Data

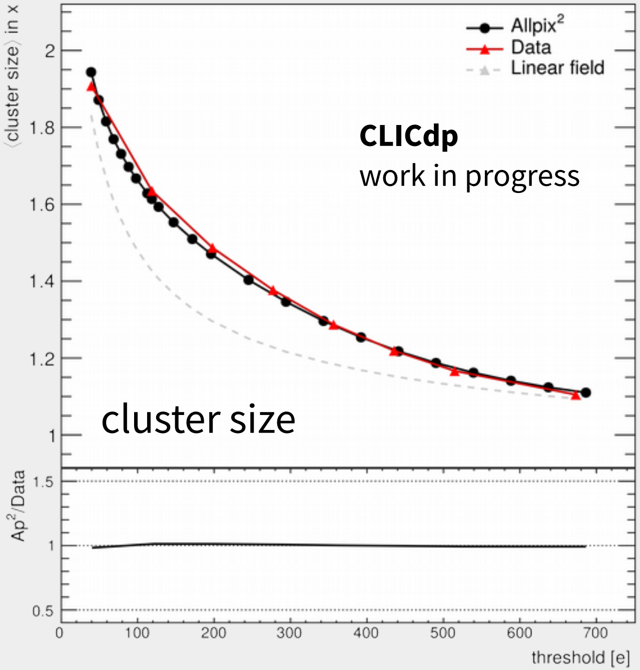


Allpix^2



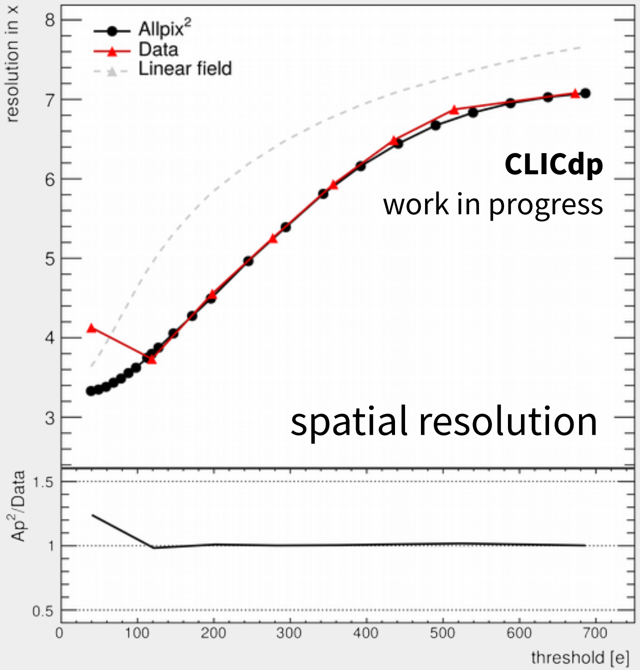
Reproducing Resolution at Different Thresholds

- Data and simulation match well, e.g. for **cluster size & resolution vs. threshold**
- Simulation with linear electric field does not describe data



CLICdp
work in progress

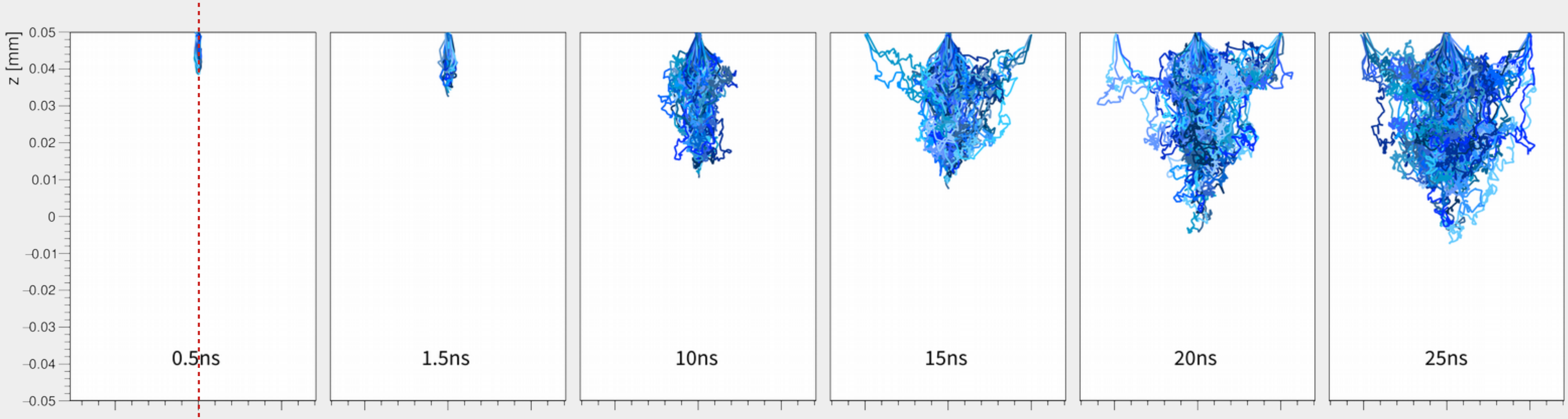
cluster size



CLICdp
work in progress

spatial resolution

Visualizing Charge Carrier Motion



- Charge carrier movements at different times after the deposition
  - Only electrons shown which reach the electrodes, holes & other electrons omitted
  - Contributions form the substrate silicon after ~10ns
  - Charge sharing visible after ~15ns

A Word On…

Development of Common Tools

```
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);

ential virtual destructor.

s 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;
```

A Word on Writing Code for MC Simulations

- Implementation of algorithms is not the most time-consuming part
- Most time-consuming part is to do it such, that the algorithms are...

  ...validated with prototype data & device simulations

  ...well documented

  ...maintainable over a period longer than O(1 fellow) / O(1 PhD)

- Development of Allpix^2: spend considerable time on
  - Writing documentation → lower barrier for new users
  - Implementing automated testing, compilation → ensure software always works
  - Code review for new features → ensure functionality/compatibility

User Manual & Code Documentation

- Focus from the very beginning on well-documented framework
- Source code documentation for every class, method
  - Doxygen markup for code reference
  - Deployed to the website for tags
- Extensive User Manual in LaTeX
  - Automatically compiled by CI
  - Module documentation as Markdown
    - Document module parameters, algorithms
    - Included in manual via Pandoc

```
namespace allpix {

    /**
     * @brief Instantiation of a detector mode
     *
     * Contains the detector in the world with
     * (like the electric field). All model spe
     * properties are stored in its DetectorMod
     */
    class Detector {
        friend class GeometryManager;

    public:
        /**
         * @brief Constructs a detector in the
         * @param name Unique name of the detec
         * @param model Model of the detector
         * @param position Position in the wor
         * @param orientation Rotation matrix
         */
        Detector(std::string name,
                 std::shared_ptr<DetectorModel
                 ROOT::Math::XYZPoint position
                 const ROOT::Math::Rotation3D&

        /**
         * @brief Get name of the detector
         * @return Detector name
         */
        std::string getName() const;
```

GenericPropagation

Maintainer: Koen Wolters (koen.wolters@cern.ch), Simon Spannagel (simon.spannagel@cern.ch)
Status: Functional
Input: DepositedCharge
Output: PropagatedCharge

Description

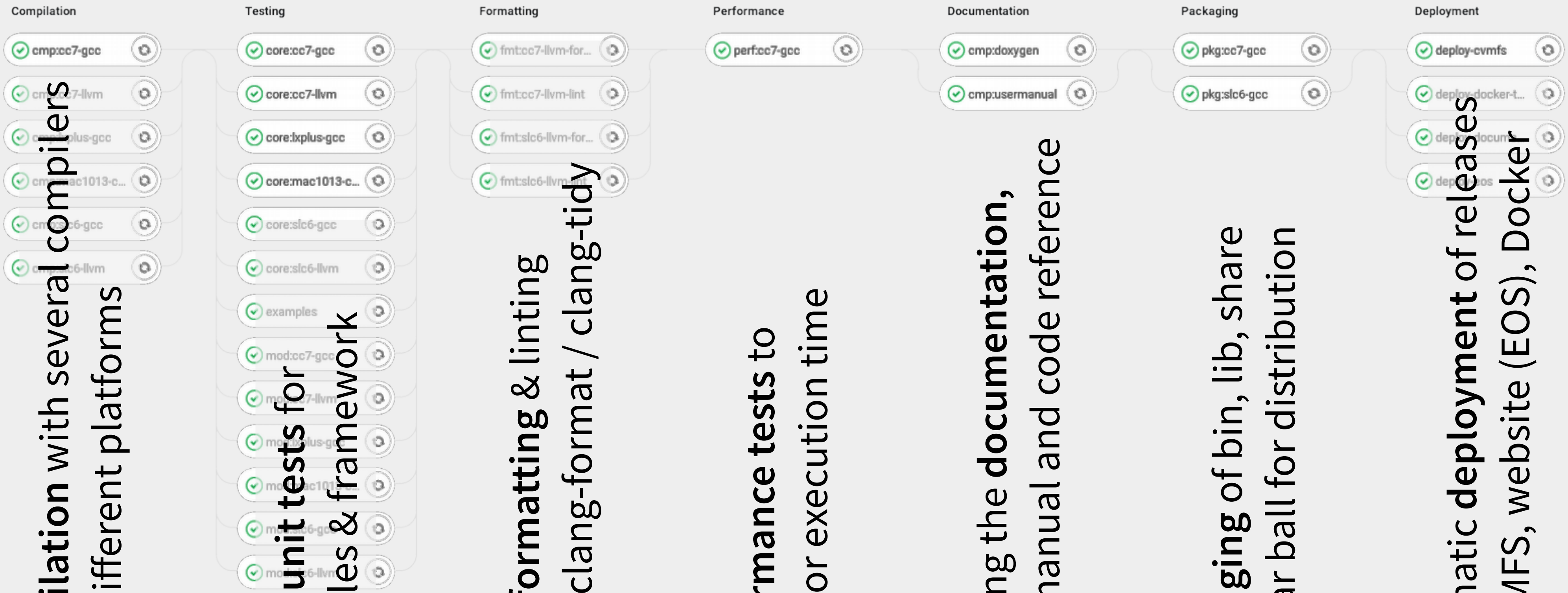
Dependencies

Parameters

Usage

```
[GenericPropagation]
type = "timepix"
temperature = 293K
charge_per_step = 25
```

Continuous Integration & Testing



compilation with several compilers
on 3 different platforms

many **unit tests** for
modules & framework

code formatting & linting
using clang-format / clang-tidy

performance tests to
monitor execution time

building the **documentation**,
user manual and code reference

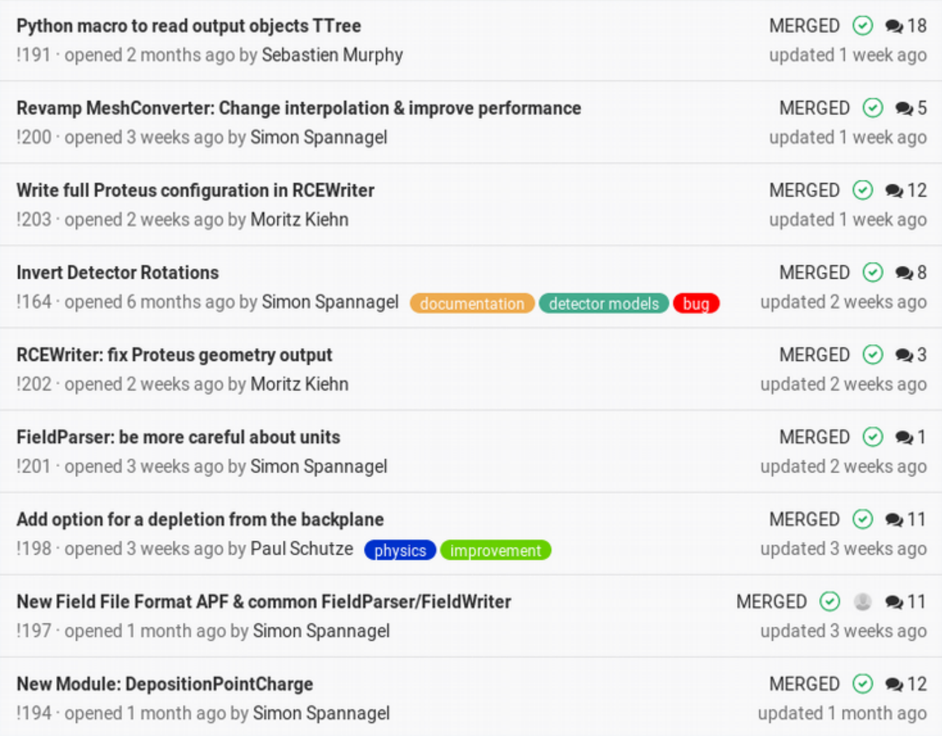
packaging of bin, lib, share
into tar ball for distribution

automatic **deployment** of releases
to CVMFS, website (EOS), Docker

Code Review via Merge Requests

- No new code lands in master without review by another party
  - Using GitLab's approval feature
  - Extensive discussions about code, but also style, naming schemes
- Proven to be **very effective**
  - Several bugs found before the merge
  - New users appreciate guidance
- Proven to be **labor-intensive**
  - Read (and understanding) every change
  - Always be supportive, positive

...just some of them



Python macro to read output objects TTree
!191 · opened 2 months ago by Sebastien Murphy
MERGED ✓ 💬 18
updated 1 week ago

Revamp MeshConverter: Change interpolation & improve performance
!200 · opened 3 weeks ago by Simon Spannagel
MERGED ✓ 💬 5
updated 1 week ago

Write full Proteus configuration in RCEWriter
!203 · opened 2 weeks ago by Moritz Kiehn
MERGED ✓ 💬 12
updated 1 week ago

Invert Detector Rotations
!164 · opened 6 months ago by Simon Spannagel documentation detector models bug
MERGED ✓ 💬 8
updated 2 weeks ago

RCEWriter: fix Proteus geometry output
!202 · opened 2 weeks ago by Moritz Kiehn
MERGED ✓ 💬 3
updated 2 weeks ago

FieldParser: be more careful about units
!201 · opened 3 weeks ago by Simon Spannagel
MERGED ✓ 💬 1
updated 2 weeks ago

Add option for a depletion from the backplane
!198 · opened 3 weeks ago by Paul Schutze physics improvement
MERGED ✓ 💬 11
updated 3 weeks ago

New Field File Format APF & common FieldParser/FieldWriter
!197 · opened 1 month ago by Simon Spannagel
MERGED ✓ 💬 11
updated 3 weeks ago

New Module: DepositionPointCharge
!194 · opened 1 month ago by Simon Spannagel
MERGED ✓ 💬 12
updated 1 month ago

Allpix² Users, Contributors

- First **user workshop** held
  26-27 November 2018 @ CERN
  Tutorials, discussions, feedback
- Increasing number of community contributions to the code base

ONERA Aerospace Lab, Toulouse
Georg-August-Universität Göttingen
University of Birmingham
University of California, Berkeley
NIKHEF, Amsterdam
University of Glasgow
Czech Techn. University, Prague
Rutherford Lab, STFC
ETH Zurich
Université de Montréal
Charles University, Prague
CLICdp @ CERN
CMS Pixel @ CERN
ATLAS Strips @ CERN
LHCb VeloPix @ CERN
ATLAS Monolithic @ CERN
IHEP Beijing
Freiburg University
Utrecht University
ATLAS @ DESY
CMS Lorentz Angle @ DESY
ELAD @ DESY
University of Liverpool
ATLAS SCT @ KEK
Dortmund University
Université de Genève
AGH University Krakau

Disclaimer: these are just some user groups we have been in contact with...

In a nutshell…

Summary

- Designing a new silicon detector is a major undertaking
- Simulations are a vital component of the prototyping effort
  - Device simulations help in understanding and optimizing the design
  - Monte Carlo Simulations are required to assess the device performance
- Models with different complexity are available

  fast & coarse ↔ slow & precise
- Including results from device simulations improves detector modeling
- **Allpix Squared**: flexible platform for implementation of different algorithms
- Extensions planned, participation from community very welcome

Allpix Squared Resources

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

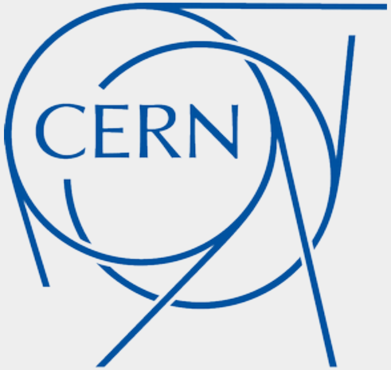
Repository
https://gitlab.cern.ch/allpix-squared/allpix-squared

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


CERN