Status update of Allpix Squared simulations for Multi-element Germanium Detectors for Synchrotron Applications

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Ref: EXP-DET22-P086-A

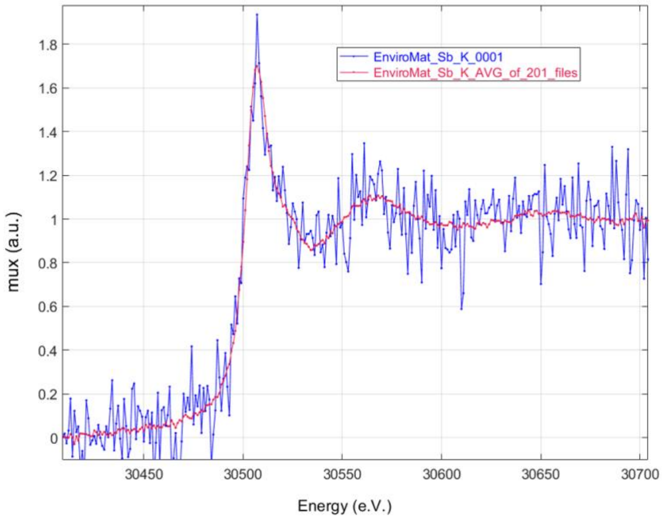
Outline:

- *Multi-element germanium detectors*
- *Motivation: charge sharing mitigation*
- *Allpix Squared simulation chain*
- *Summary & next steps*

Multi-element germanium detectors

Motivation for synchrotron techniques:

- Detection of tender and hard X-rays (**20-100 keV**)
- **Environmental science**: detection of fluorescence lines of polluting traces (Cd, Mo, Sb) in soil
- Three key features for detection sensitivity:
  - **Maximum input count rate** -> **Multi-element sensor**
  - **Signal-to-background ratio** -> **Charge sharing mitigation**
  - **Energy resolution** -> **Charge sharing mitigation**

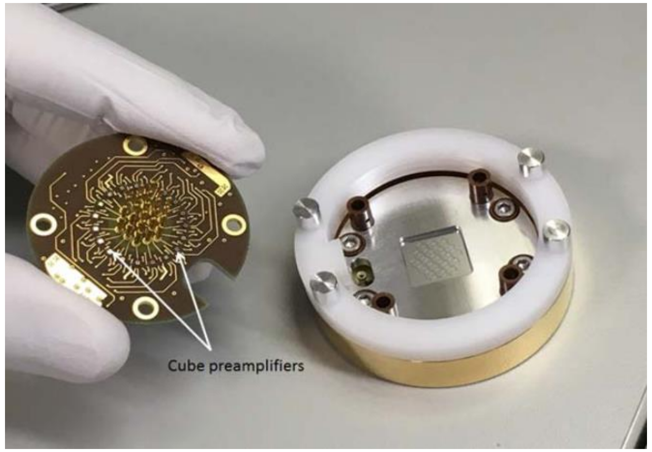


XANES + 1st part of EXAFS of Sb in soil for comercial germanium detector (1 vs 200 runs)

F.J. Iguaz *et al.*, *proceeding of SRI2021 conference*
https://arxiv.org/abs/2204.07490

R&D projects at SOLEIL synchrotron:

- **DLS-SOLEIL collaboration (2019-2022):**
  - Hole collection germanium, 19 hexagonal pixels (Ø 2 mm)
  - Development of a new front-end board in ceramics
  - First demonstrator tests in April 2022
- **XAFS-DET project (2021-2024):**
  - Working package of the EU project INFRA-INNOV-2020 (LEAPS-INNOV consortium)
  - Hole collection germanium, 10 non-identical pixels
  - Development of a new multi-channel low-noise CMOS preamplifier



Demonstrator of DLS-SOLEIL collaboration

https://doi.org/10.1109/TNS.2020.3004923

Simulations used to study the detector performance

Charge sharing events

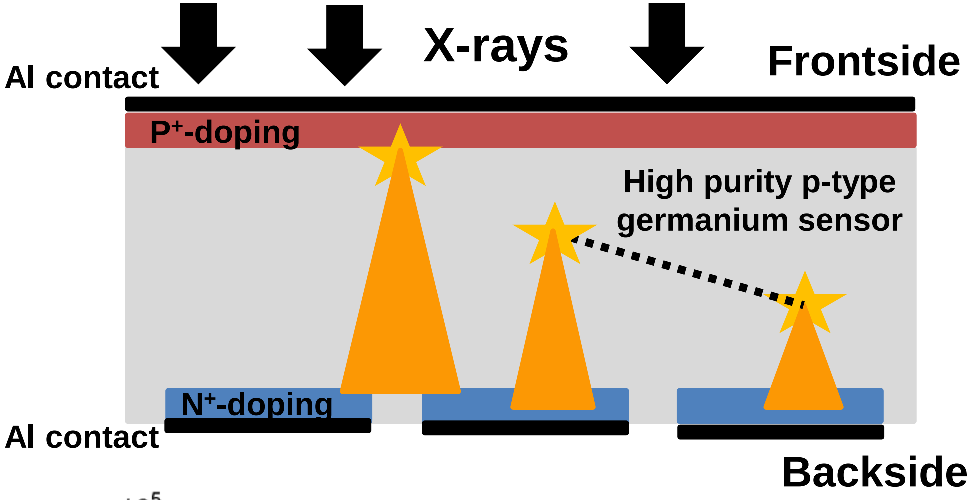
Definition: Events where the initial X-ray energy is shared between neighbouring pixels.

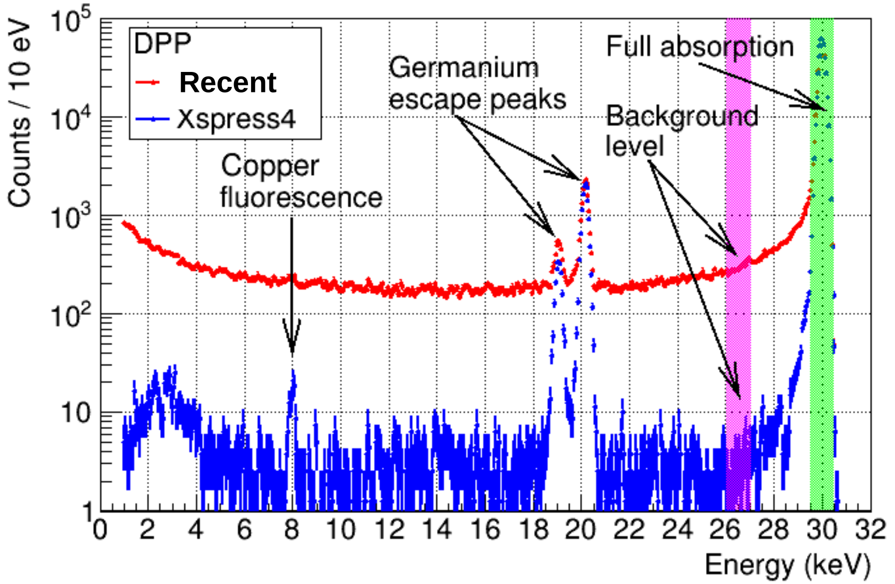
Physical origin:

- **Split events:** charge carriers created by impinging X-rays at the detector frontside spread over multiple neighbouring pixels when drifting to backside pixels
- **Fluorescence events:** two well-separated energy deposits which spread over multiple pixels

Bad consequences:

1. Intensity reduction of the fluorescence signal line (S)
2. Increase of the background level (B), which comes essentially from the Compton level of high energy lines
3. Degradation of signal-to-background (S/B) ratio
4. Degradation of the energy resolution





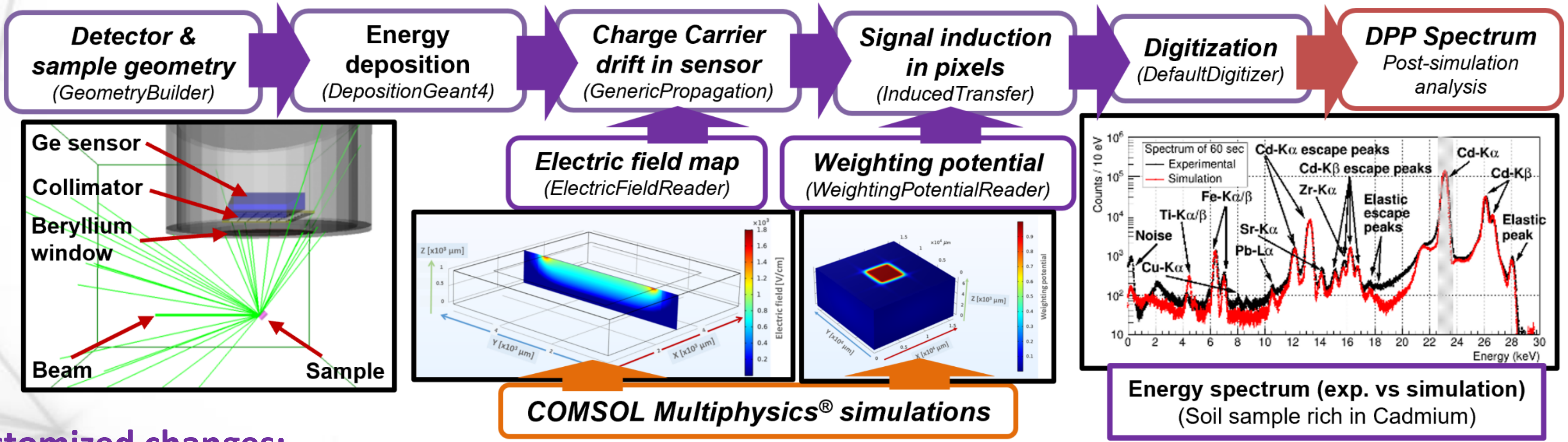
Energy spectrum of direct 30 keV X-ray beam in a multi-element germanium detector

Strategies for charge sharing mitigation

1. **Metal collimator/mask at the frontside of the germanium sensor**
   – Strategy used in current commercial detectors (Titanium collimator coated with aluminum)
   – Very effective for low energy X-rays (< 30 keV)
   – **Main issues:**
     - Significant reduction of the detection active area (~30% for 5 mm-length square pixels)
     - Not realistic for small pixel sizes
2. **Charge sharing events rejection by Digital Pulse Processor (DPP) firmware**
   – Strategy of the next-generation DPP, like Xspress4
   – Very effective in a wide energy range (0-40 keV)
   – Reduction of detector efficiency, but this is not an issue for synchrotron techniques
3. **Initial X-ray energy reconstruction by DPP firmware**
   – Strategy of multi-element CdTe detectors in Astrophysics
   – **Main issue:** energy resolution degradation, if several pixels are combined

➡ Current simulation work compares the detector performance results of the two first strategies

Allpix Squared simulation chain



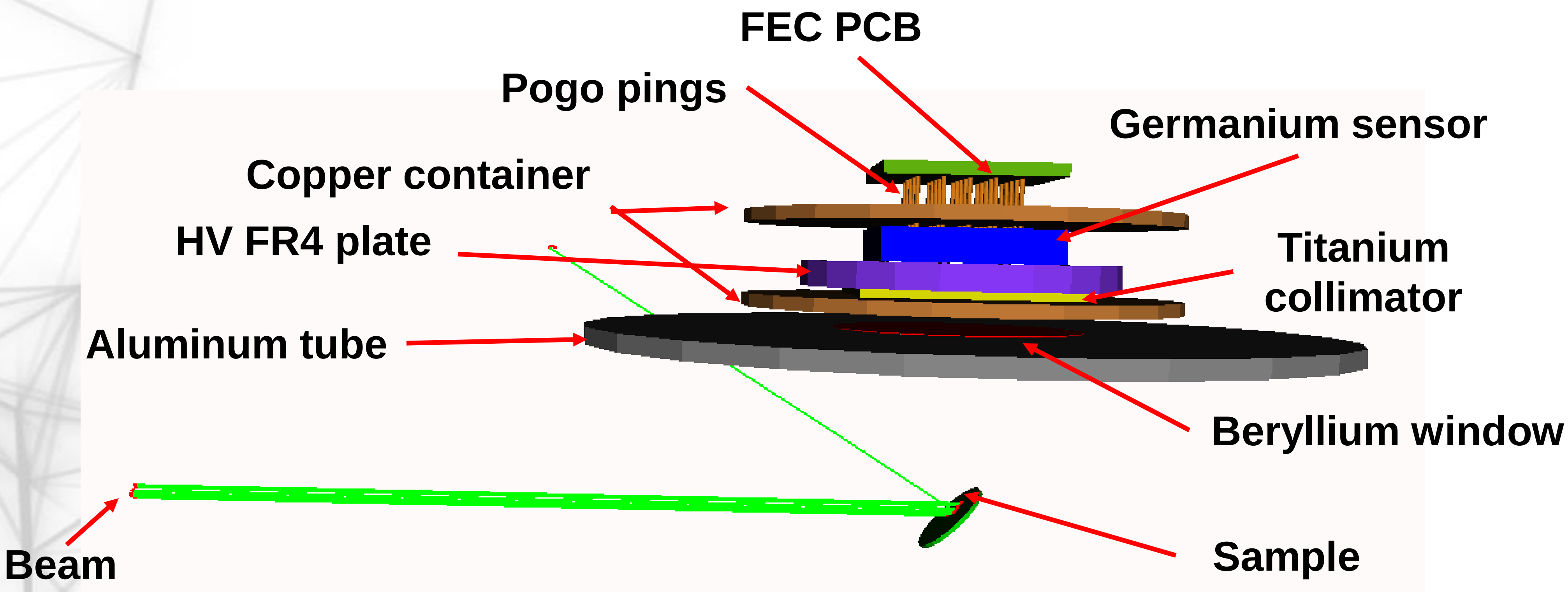
T. Saleem *et al.*, *JINST* **17** (2022) P02013
https://doi.org/10.1088/1748-0221/17/02/P02013

Customized changes:

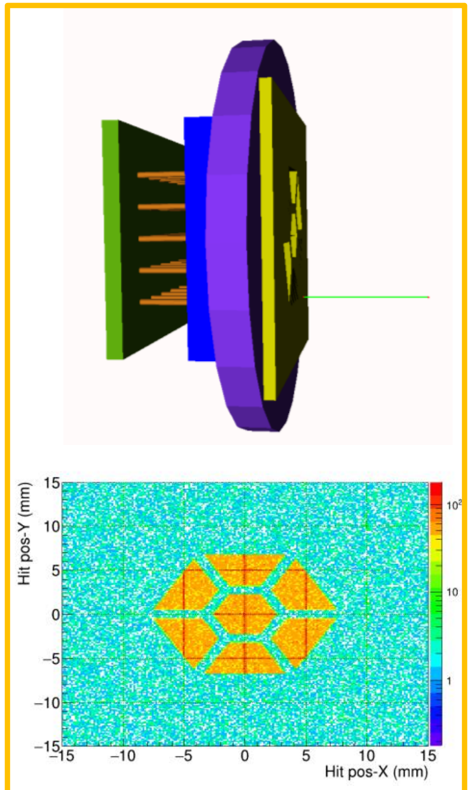
- **GeometryBuilder:**
  - Germanium material for the sensor -> **Sensor material (v2.3)**
  - Detector & sample passive materials -> **GDML passive volume (v2.2)**
- **DepositionGeant4:**
  - Electron-hole pair energy & Fano factor -> **Sensor material (v2.3)**
  - Physics list for X-ray polarization (*G4EmLivermorePolarizedPhysics*) -> **Not predefined name in Geant4**
- **GenericPropagation:**
  - Jacoboni-Canali model for germanium -> **Sensor material (v2.3)**

Simulation jobs:
- *SOLEIL cluster called SUMO*
- *French TGCC facility (TOPAZE)*

Detector geometry



- In the past, the detector geometry was implemented directly in the code.
- Since the release 2.2 (28 Feb 2022), the geometry is implemented as passive volume in GDML format in module *GeometryBuilderGeant4*.
- Example code is available in:
  - https://allpix-squared-forum.web.cern.ch/t/geometrybuildergeant4-module-passive-volumes-in-gdml-question-issue/275

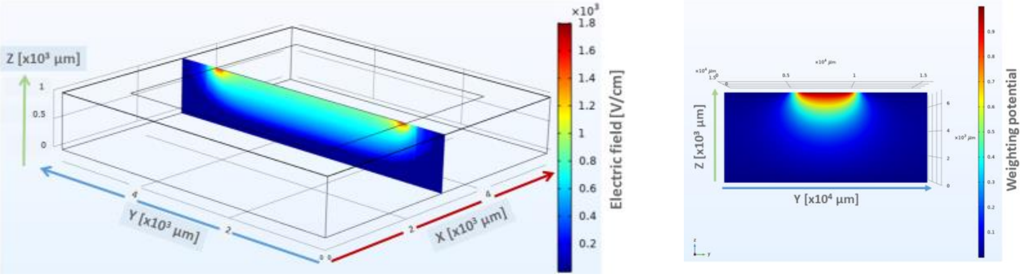


Example of titanium collimator

3D maps of electric field & weighting potential

COMSOL Multiphysics® + Semiconductor module

- Commercial software
- Finite Element Method (FEM), **fixed grid**
- **Application**: Square pixels (5 mm x 5 mm)
- **Problem: Time** for convergence **very long** for large sensors (optimized for µm devices) -> Not useful for R&D requiring to simulate different configurations



T. Saleem *et al.*, *JINST* **17** (2022) P02013
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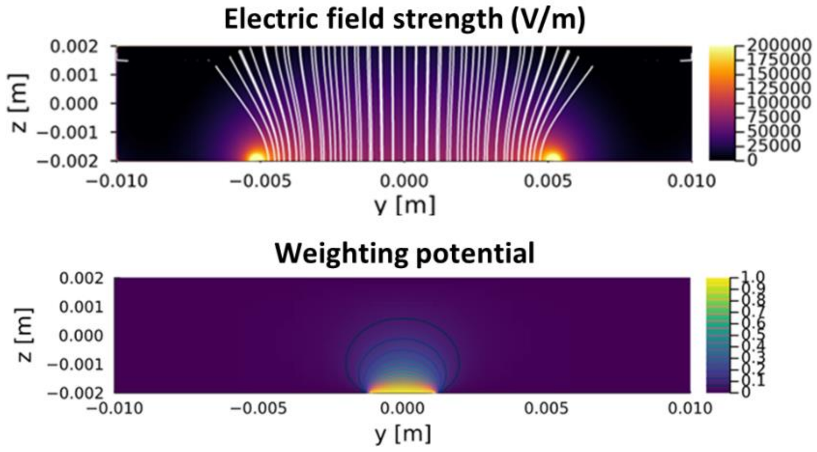
SolidStateDetectors (SSD)

https://github.com/JuliaPhysics/SolidStateDetectors.jl
https://iopscience.iop.org/article/10.1088/1748-0221/16/08/P08007

- Developed by LEGEND collaboration
- Successive over relaxation (SOR) method, **adaptative grid**
- **Application**: Hexagonal & trapezoidal pixels
- Major advantages:
  - Optimized for **large germanium sensors with contacts of arbitrary geometry**
  - Optimized for **parallel computing**
  - The whole simulation chain can be developed with the same package (good to cross-check simulation results)



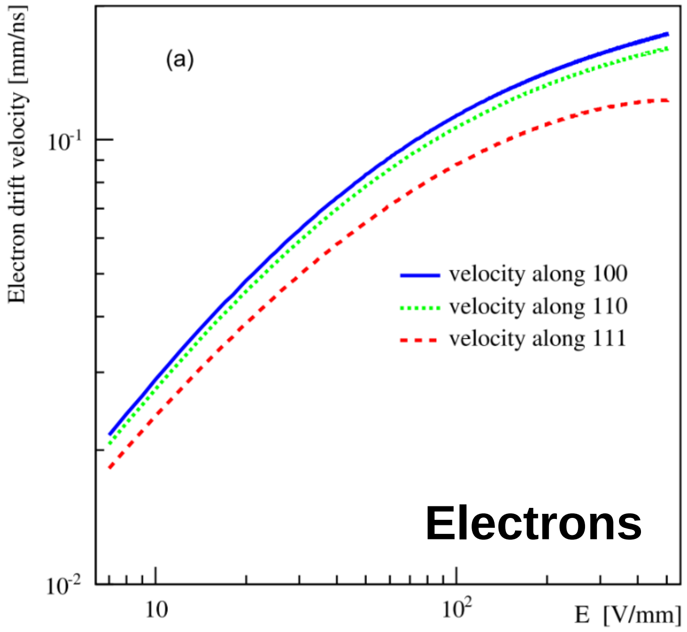
3D maps simulation for XAFS-DET project

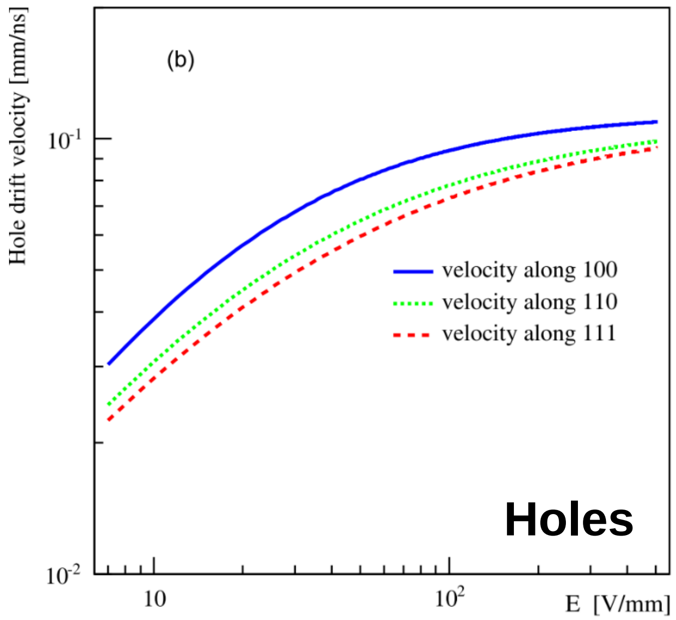
Charge Carrier drift

Table 1 Parameters for the experimental drift velocities in the ⟨111⟩ and ⟨100⟩ directions used in the simulation

Carrier	Axis	μ_0 [$\frac{cm^2}{V \cdot s}$]	$\mathcal{E}_0$ [$\frac{V}{mm}$]	β
e	⟨111⟩	38536	53.8	0.641
	⟨100⟩	38609	51.1	0.805
h	⟨111⟩	61215	18.2	0.662
	⟨100⟩	61824	18.5	0.942

$$v_{e/h} = \frac{\mu^0_{e/h} E(x)}{[1 + (\frac{E(x)}{E_0})^\beta]^{1/\beta}},$$





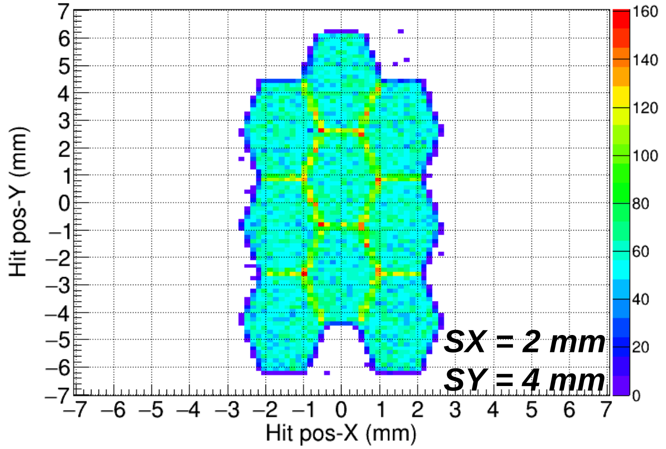
I. Abt et al., Eur. Phys. Jour. C ***68*** *(2010) 609-618*

- Modified Jacoboni-Canali model for germanium sensor along the crystallographic axis < 1 0 0> implemented in Allpix Square framework
- No big difference in drift velocity between axis -> To be validated in future with real sensor pulses
- Values for new Allpix Squared release to be checked

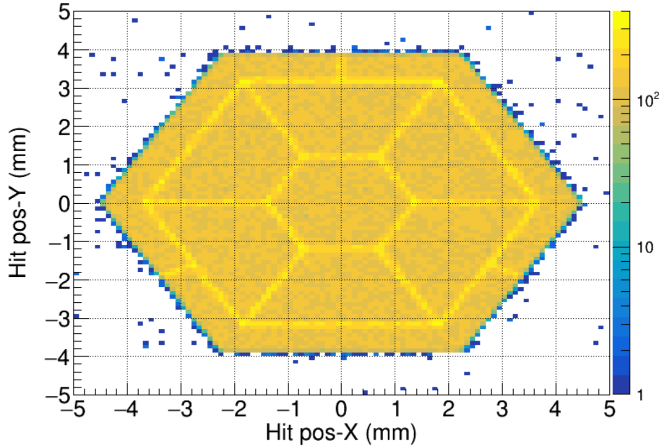
Sensor pixelization

- First simulation work used **squared pixels**
  - 5 mm pitch, 4.2 mm implant length
  - T. Saleem *et al.*, *JINST* **17** (2022) P02013
- Current simulation work for R&D projects needs:
  - 19 hexagonal pixels, for DLS-SOLEIL project
  - Non-identical pixels (1 hexagon, 6 trapezoids, 3 rings), for XAFS-DET project
- **Hexagonal pixels:**
  - Work made by Ryuji Moriya (CERN Summer student) & Simon Spannagel to implement hexagonal pixels
    - Support for Hexagonal Pixels and Grids (!539) · Merge requests · Allpix Squared / Allpix Squared · GitLab (cern.ch)
    - Code downloaded & tested -> **It works fine for us ☺**
  - However, a correct wrapping and lookup of fields is missing
    - DetectorField: Perform Field Lookup on Per-Pixel Basis (!560) · Merge requests · Allpix Squared / Allpix Squared · GitLab (cern.ch)
    - This is necessary for using precise 3D maps -> **We would like to use it!**
- **Non-identical pixels:**
  - Email to Simon: "*Not straightforward but it could be implemented as another detector model*" -> **To be studied in future**

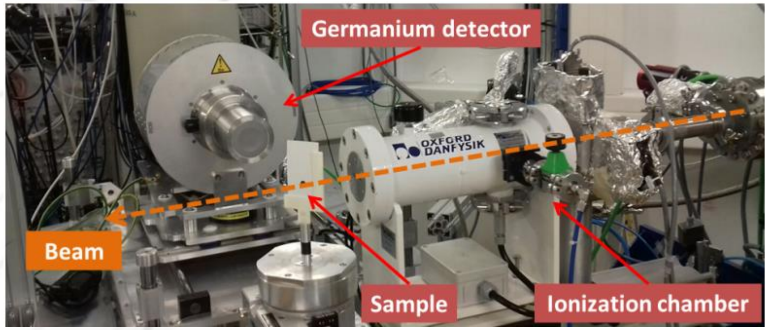
Hexagonal pixels (Flat type)

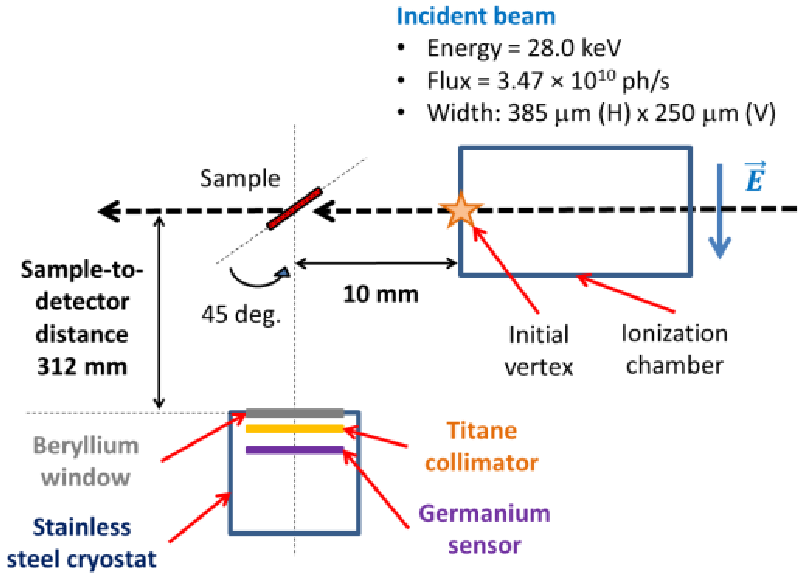


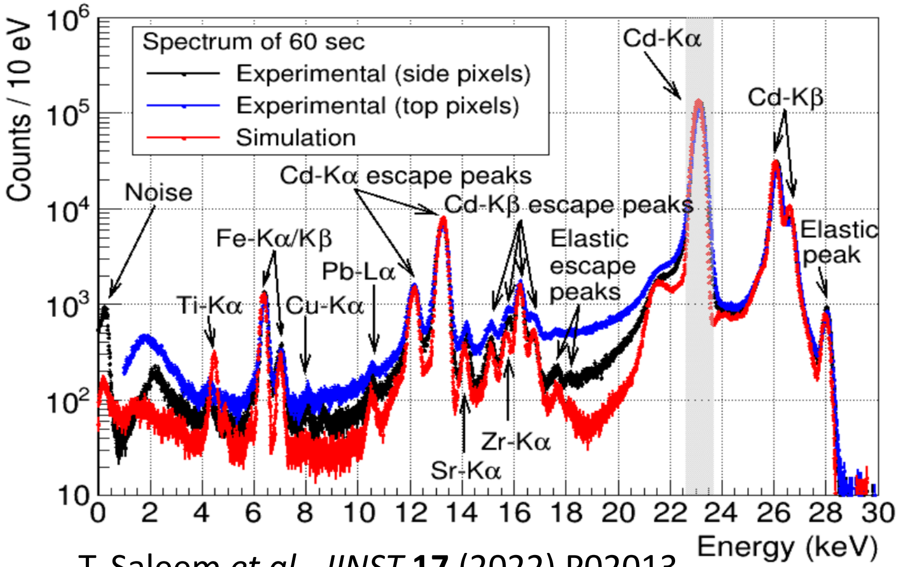
XAFS-DET pixel configuration



Simulation vs experimental data







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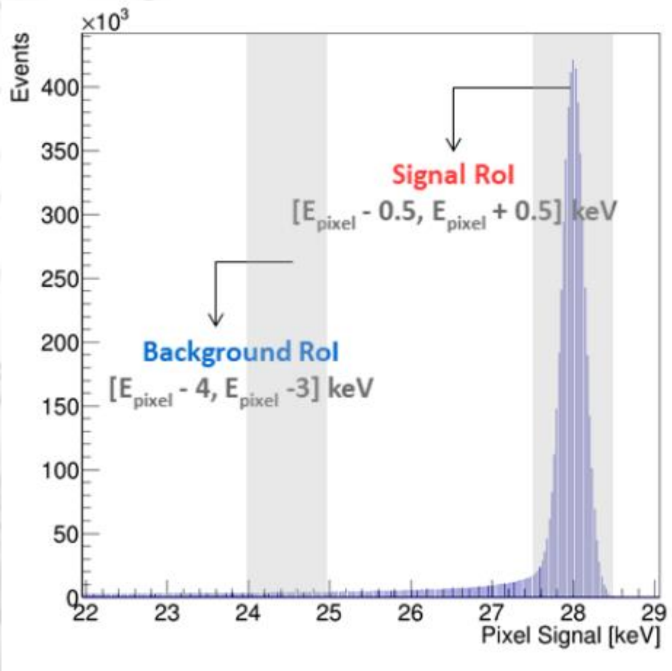
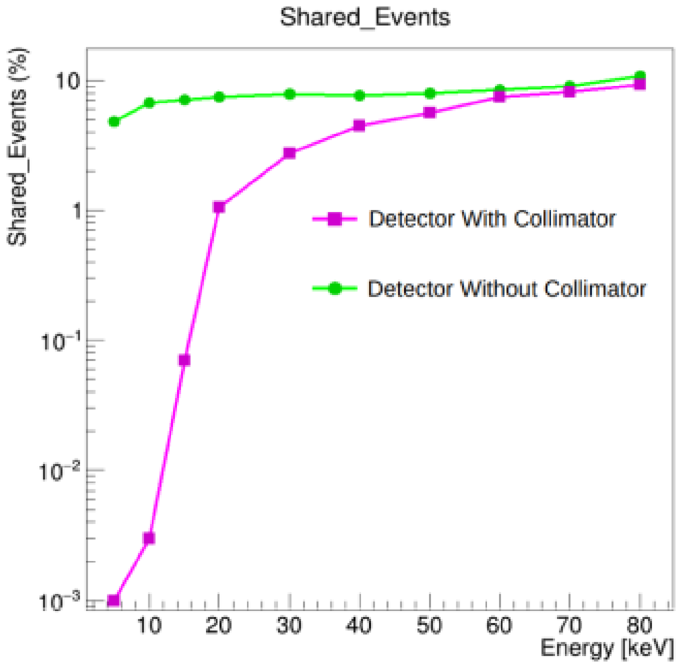
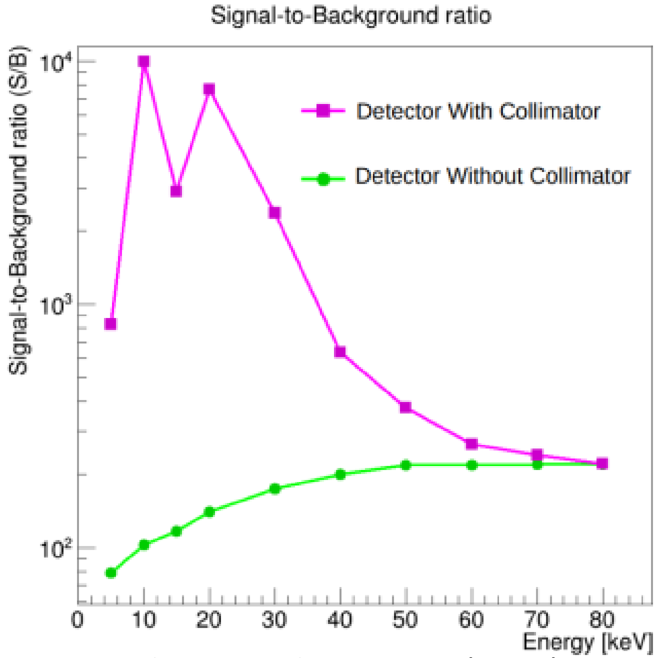
- XAFS experimental data provided by SAMBA beamline used to set up the simulation chain
- **Detector**: commercial 36 element germanium detector + XIA-XMAP DPP.
- **Experimental data:** organic soil rich in cadmium, fixed beam energy (28 keV), 60 sec spectra.
- Comparison of simulation and experimental spectra:
  - **Fair agreement**, especially for the X-ray emission lines of the elements.
  - **Higher Compton level** (2-21 keV) -> Level correlated to the distance to two disconnected pixels (detector problem)
  - **Presence of titanium fluorescence lines** -> Aluminium coating of collimator to be implemented in detector model

Direct beam performance







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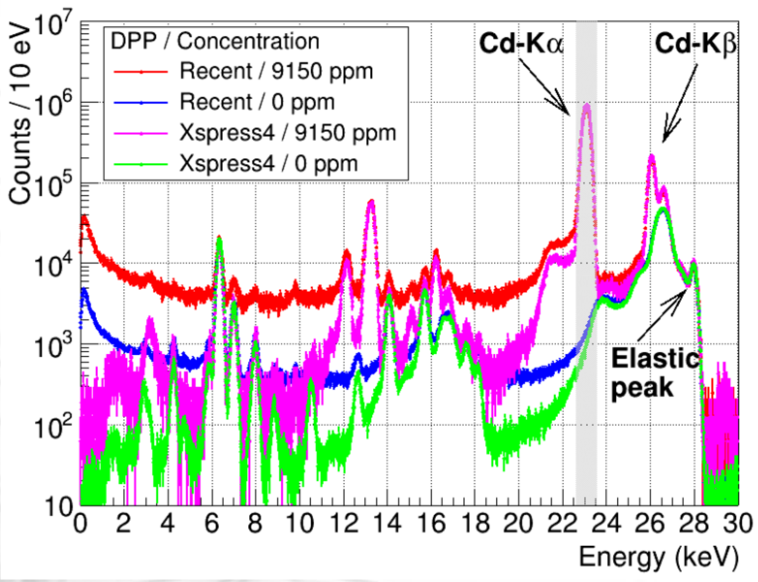
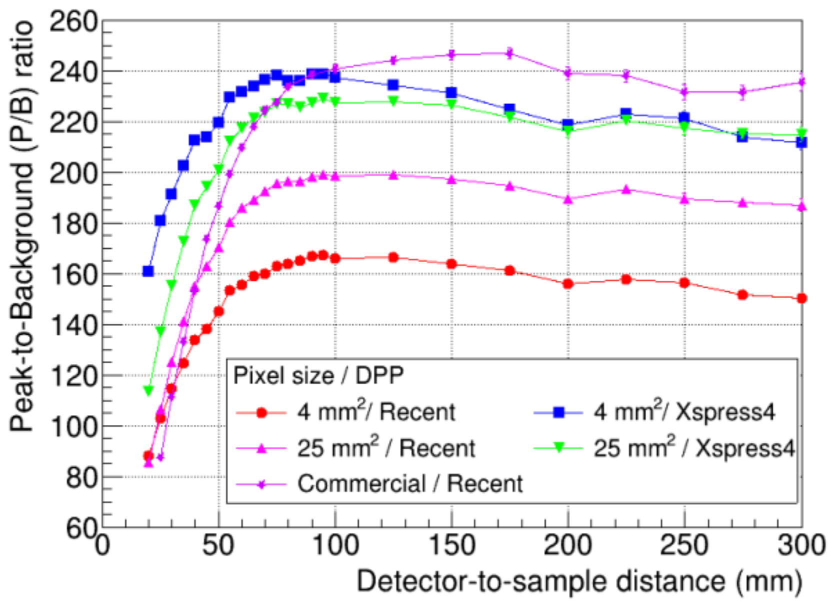
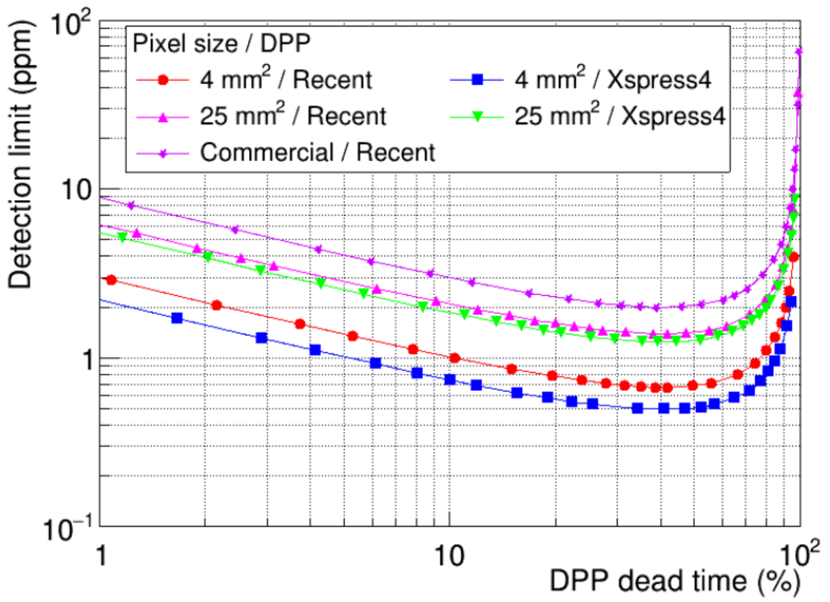
- The performance of the commercial detector to direct X-ray beam has been simulated, with and without collimator. The impact of the Digital Pulse Processor has not been considered.
  - **Signal RoI:** incident photon beam energy
  - **Background RoI:** Compton level close to the signal RoI (first approximation)
- Detector equipped with a collimator: reduction of charge sharing events and increase of S/B ratio for X-rays with energy below 30 keV.
- The detection area is increased by 30% in absence of collimator.

Detection limit of future detectors







F.J. Iguaz *et al.*, *proceeding of SRI2021 conference (28th March – 1st April 2022)*
https://arxiv.org/abs/2204.07490

- Detection limit to cadmium traces in soil of a XAFS experiment with a multi-element germanium detector.
- Configurations: 1) two pixel sizes (4 & 25 mm^2), 2) recent DPP or future Xspress4
- First results using linear electric field approximation in sensor & perfect pixel transfer
- Very small pixels combined with Xspress4 DPP could increase the sensitivity to pollution traces **a factor 4** compared to current detectors (**a factor 16** in exposure time)

Summary

Conclusions:

- Complete and operational simulated chain based on Allpix Squared framework, customized to multi-element germanium detectors & XAFS experiments, has been built
- Simulated 3D maps of electric field & weighting potential using COMSOL Multiphysics® or SolidStateDetectors have been exported to Allpix Squared framework
- Experimental data of SAMBA beamline has been used to set up & validate the simulation chain
- First detector performance studies have been made

Next steps:

- To finish a sensibility study for germanium detector with square pixels (two different sizes) & no collimator using 3D maps simulated by SolidStateDetectors
- Evolution of Allpix Squared in a very near future to take into account pixels with different geometries and sizes ?
  - This is being done now using SolidStateDetectors package + customizations

Thanks for you attention. Questions?