Allpix-Squared Simulations of Multi-element Germanium Detectors for Synchrotron Applications

Tasneem SALEEM

SOLEIL Synchrotron – Detector Group

Allpix-Squared workshop

17th - 19th August 2021, ZOOM

Outline

- Introduction
- Customized allpix-squared version: Recent Developments on germanium detectors
- Examples: Detector Performance Studies
- Summary

Introduction

<u>**Multi-element Germanium Detector R&D:**</u>

- *SOLEIL* is a third generation light source, with nominal beam energy 2.75 GeV and 29 beamlines

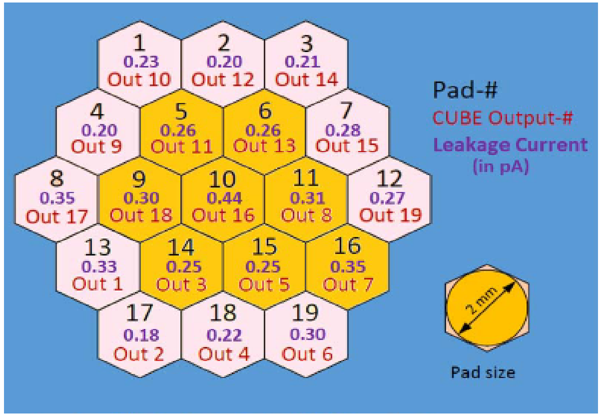
- *Detector group* at SOLEIL is largely involved in R&D of new generation of High Purity Germanium (HPGe) detector for future Synchrotron application

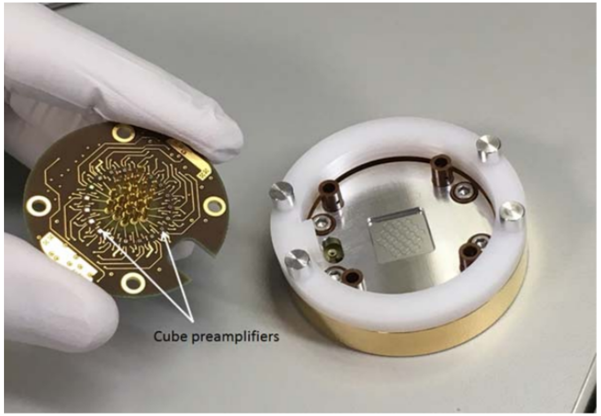
- Next generation of X-ray detectors *requirements*:

  - Analyse chemical species with very low concentrations (<<10 ppm)
  - Cope with the very high photon flux (10^{11} ph/s) and input count rate (10^3 kcps)

- Hexagonal Pixel Multi-element HPGe is a promising candidate:

  - New monolithic Ge sensor composed of 19 hexagonal pixels of 2 mm inner diameter
  - Maximize compactness and granualrity of tradiational detectors





Motivation

Multi-element Germanium Detector R&D:

- More info is needed during development and testing:

  - Details of electric field for optimised charge collection on the collection implant.
  - Optimal sensor thickness, pixel size, pixel shape, inter-pixel region width
  - Design with/out collimator
  - Charge sharing effect
  - ...

→ need for modular, detailed simulations of the germanium sensors with rapid feedback

- A special derivation of allpix-sqaured has been developed including:

  - New material, germanium, with its corresponding mobilities
  - New geometries: hexagonal pixel shape

Customised Allpix-squared

New Material – New Mobilities:

Modification Description	Module	Replacment
Sensor, Pixel & Chip material	GeometryBuilderGeant4	“Silicon” → “germanium”
Fano Factor	DepositionGeant4	Si: 0.115 → Ge: 0.112
Charge Creation Energy	DepositionGeant4	Si: 3.64 → Ge: 2.62
Mobility* and diffusion parameters	GenericPropagation	Temperature_ = 77.36;

- Empirical values of parameters taken from literature:

```
electron_Vm_ = Units::get((38536.0 * 53.8 * 10.0), "cm/s");
electron_Ec_ = Units::get((53.8 * 10.0), "V/cm");
electron_Beta_ = 0.641;

hole_Vm_ = Units::get((61215.0 * 18.2 * 10.0), "cm/s");
hole_Ec_ = Units::get((18.2 * 10.0), "V/cm");
hole_Beta_  = 0.662;
```

* R. Quay et al., "A Temperature Dependent Model for the Saturation Velocity in Semiconductor Materials," Materials Science in Semiconductor Processing,vol. 3, no. 1-2, pp. 149-155, 2000.

Customised Allpix-squared

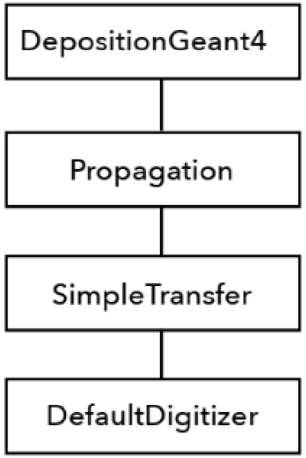
New Geometries - Hexagonal pixels:

- Idea:

  - Keep the cartesian coordinate system inside the sensor.

  - Change from cartesian to hexagonal coordinate system when simulated particles reach a collection mode

  → thanks to K. Dort !



- Implement function "getPixelIndex()" into DetectorModel to check pixel index for any module

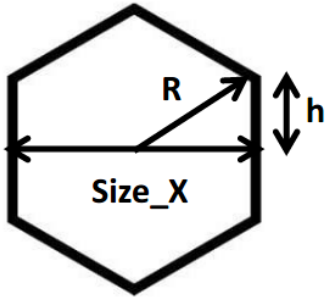
```
virtual ROOT::Math::XYVector getPixelIndex(const ROOT::Math::XYZPoint & position) const {
      double xpixel = static_cast<int>(std::round(position.x() / getPixelSize().x()));
      double ypixel = static_cast<int>(std::round(position.y() / getPixelSize().y()));
        return {xpixel, ypixel};
```

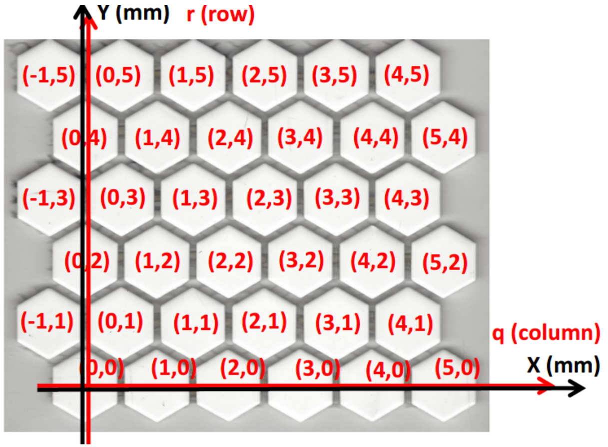
Customised Allpix-squared

New Geometries - Hexagonal pixels:

- Implement new detector module: HexagonalPixelDetectorModel, and define new coordinate (radius,height)

```
ROOT::Math::XYVector getPixelIndex(const ROOT::Math::XYZPoint & position) const override
{
        double sizex = getPixelSize().x();
          double radius = std::sqrt(3)/3.0 * sizex;
          double height = 0.5 * radius;
```



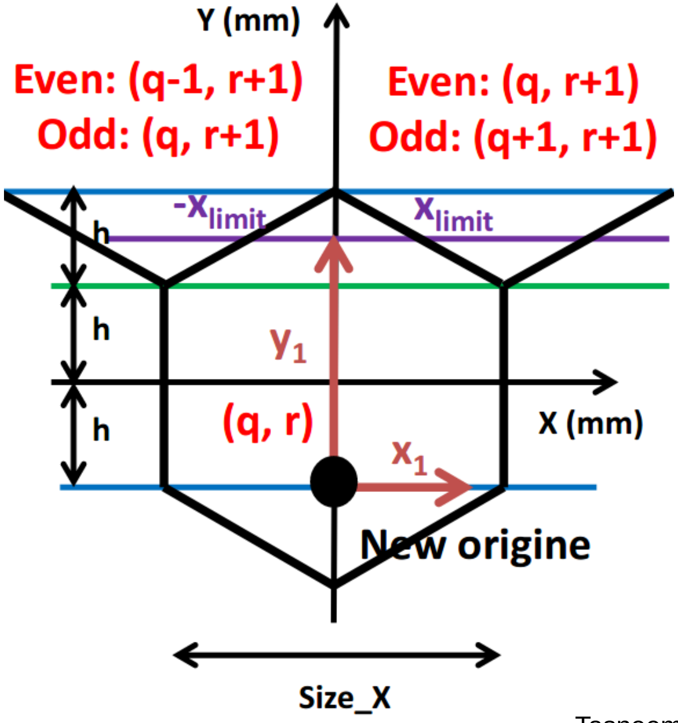


Customised Allpix-squared

New Geometries - Hexagonal pixels:

- Define algorithm to find the nearest pixel at position (x,y)

From F. Iguaz



$$x_1 = x - r \times Size\_X - {}^{Size\_X}/_2$$

$$y_1 = (y + height) - r \times (3 \times height)$$

- If $y_1 < (2 \times \text{height})$, we are in the first case, i.e., (q,r) as before.
- If $y_1 > (2 \text{ x height})$, I calculate:

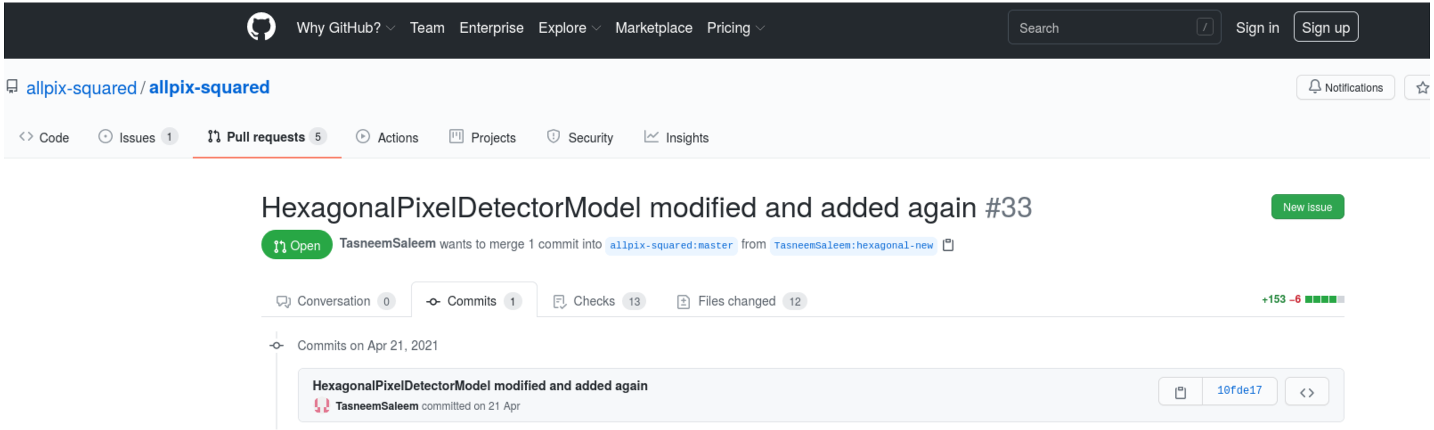
$$x_{limit} = \frac{Size\_X}{2} \times \frac{3h - y_1}{h}$$

- If x > xlimit, (x,y) is in right pixel.
- If x < -xlimit, (x,y) is in left pixel.
- Otherwise, (x,y) is in central pixel

Customised Allpix-squared

New Geometries - Hexagonal pixels:

- More details are available on the hexagonal pixel branch on github:

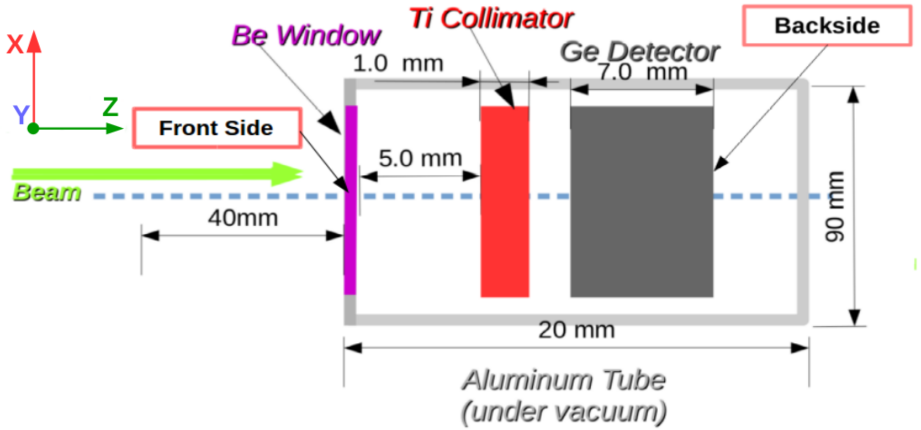


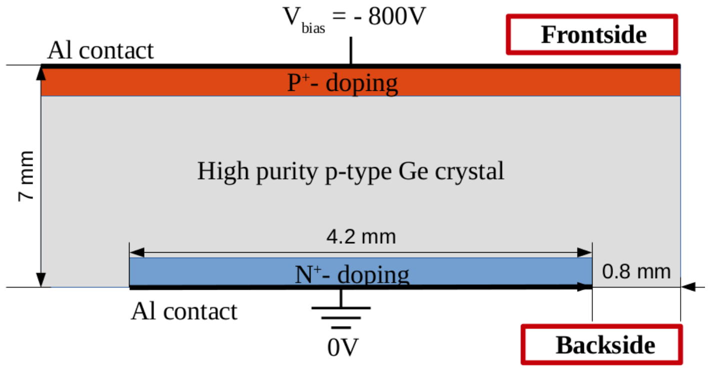
https://github.com/TasneemSaleem/allpix-squared/tree/hexagonal-branch

Case Study (1)

Conventional multi-element Ge detector

- Simulation of a multi-element germanium detector, currently in-use at SAMBA beamline.



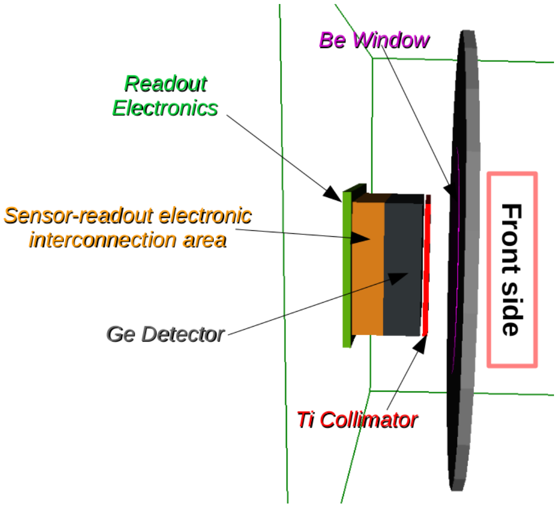


- Detector composed of:

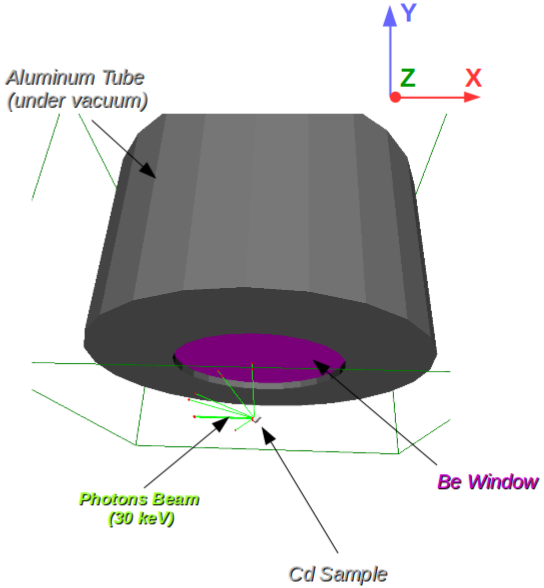
- High purity germanium crystal: 30 mm x 30 mm, 7 mm thick, 4.2 x 4.2 mm^2 pixel size, 6 x 6 pixel Matrix.
- Titanium collimator: 4.2 mm hole size, 5 mm pitch, 1 mm thick
- Aluminum cryostat: 90 mm diameter, 2 mm thick
- Beryllium window: 125 µm thick, 46 mm diameter

Conventional multi-element Ge detector

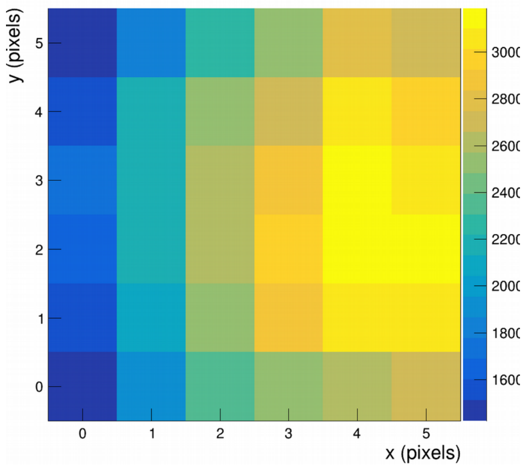
Results:



Side view of the detector geometry showing different components



A global view of the beamline showing this time the external Al tube.



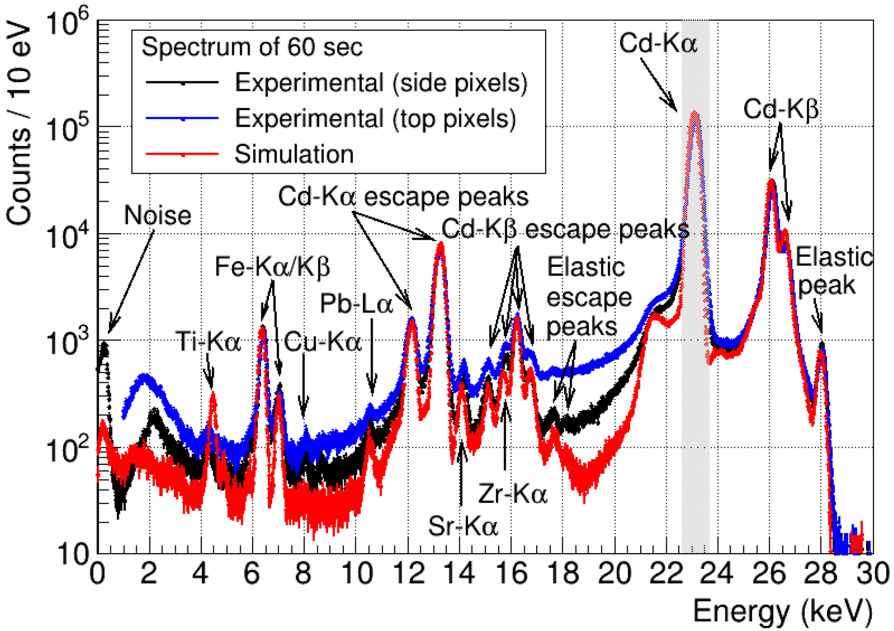
Hit map of the 6 x 6 pixel matrix

- Started with V1.4, having implemented all additional objects such as collimator, surrounding tubes, etc...
- Since V1.6, new features of passive objects can be very useful in such cases.

Conventional multi-element Ge detector

Results:

More results: arXiv:2106.11708



PREPARED FOR SUBMISSION TO JINST

Allpix-Squared Simulations of Multi-element Germanium Detectors for Synchrotron Applications

T. Saleem,[a,1] F.J. Iguaz,[a] F. Orsini[a]

[a]*SOLEIL Synchrotron, L'Orme des Merisiers, Saint-Aubin BP 48, Gif-sur-Yvette, 91190 France*

E-mail: tasneem.saleem@synchrotron-soleil.fr

ABSTRACT: X-rays spectroscopy experiments at synchrotron facilities were limited for many years by the maximum input-count rate and the signal-to-background ratio of germanium fluorescence detectors. These limitations are in part related to the germanium semiconductor device, and more generally depending on the detector (sensor) configuration and its response to the incident photon flux at different energies. In order to understand and quantify such limitations, physics simulation of the detector response is a powerful tool to provide guidelines for designing, prototyping and improving detectors, as well as modelling experimental environments, which reduces time and cost of development. For this purpose, a full-simulation chain, based on validated well-known simulation codes, has been implemented and adapted to germanium parameters. This simulation chain and specific detector performance studies, including quantification of charge sharing, as well as signal-to-background ratio at different energies, are presented in this paper. Moreover, the simulation chain is calibrated and validated using experimental results obtained at one of the beamlines at SOLEIL Synchrotron.

KEYWORDS:
X-ray detectors
Instrumentation for synchrotron radiation accelerators
Detector modelling and simulations I (interaction of radiation with matter, interaction of photons with matter, interaction of hadrons with matter, etc)
Detector modelling and simulations II (electric fields, charge transport, multiplication and induction, pulse formation, electron emission, etc)

[1]Corresponding author.

- Simulated and measured energy spectrum from the on-beamline measurement with Cd sample at the SAMBA beamline.

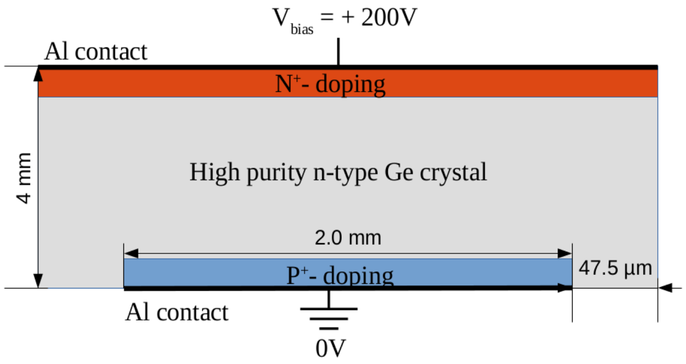
- The different fluorescence peaks from the Cd sample and the elastic peak.

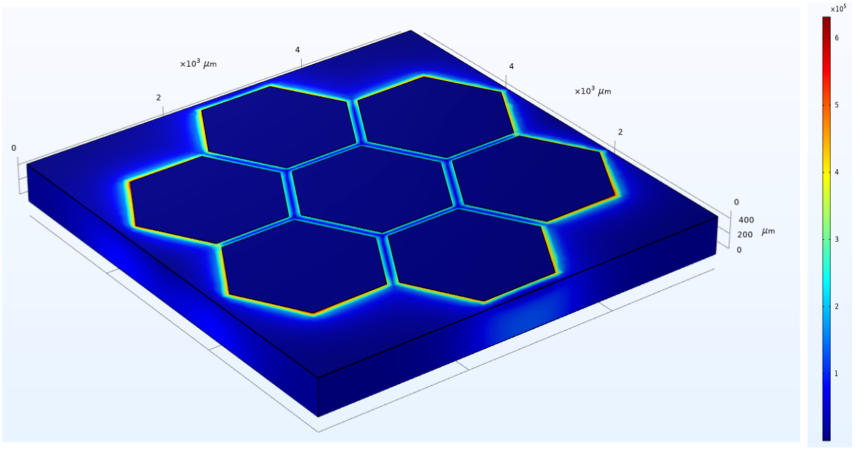
- Fair agreement between simulation and data

Study Case (2)

Hexagonal multi-element Ge detector

- Simulation of a hexagonal multi-element germanium detector

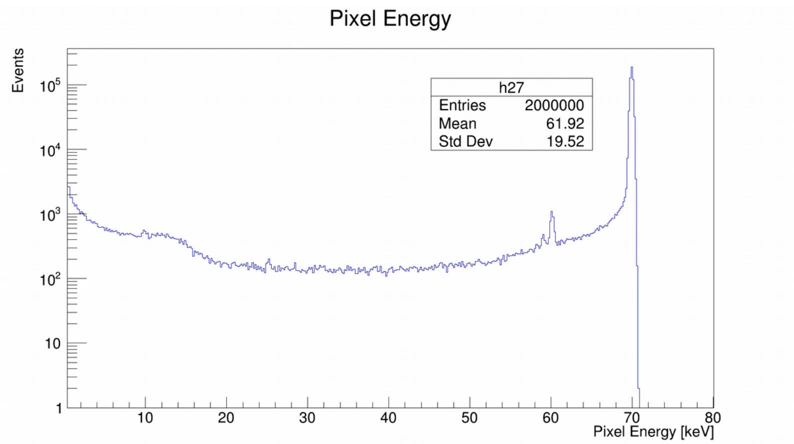


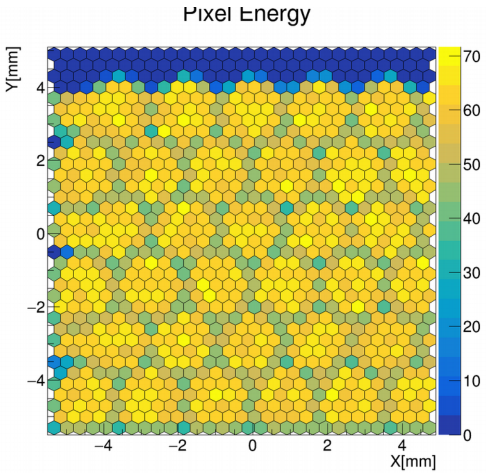


- Using the same detector configuration, but with hexagonal pixel shape
- Visualization of COMSOL simulated electric field map in 3D for the hexagonal pixel design shows one central pixel and six adjacent pixels around.
- 3D electric field map is exported to allpix-squared framework for further studies.

Hexagonal multi-element Ge detector

- Detector Response:

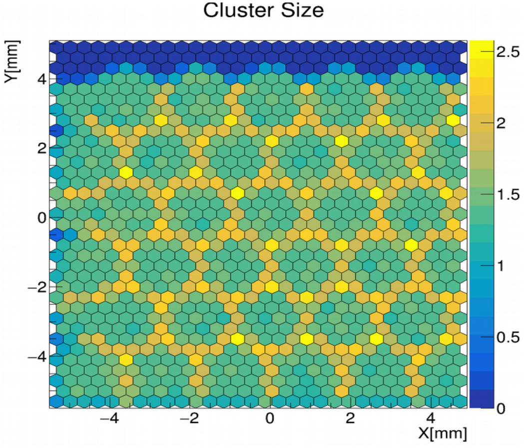


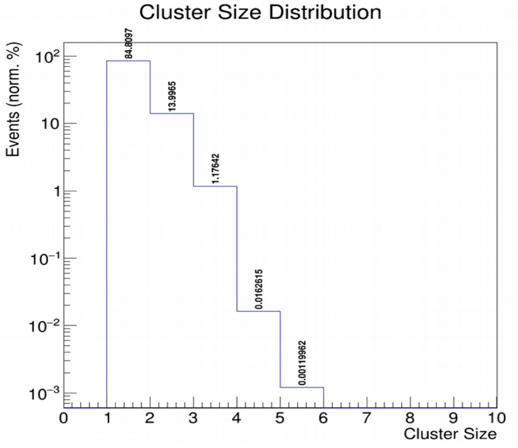


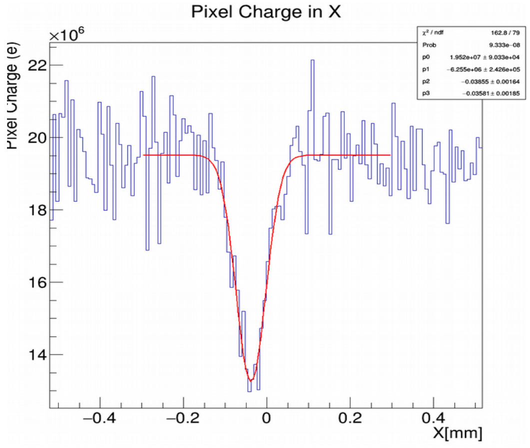
- Photon beam of energy 70 keV, perpendicular to the detector surface
- Energy spectrum shows the photoelectric peak of Ge @ 70 keV and the escape peaks of Ge @ 60 keV and 59 keV.
- Pixel energy spatial distribution shows that hexagonal pixel shape implementation is working well.

Hexagonal multi-element Ge detector

- Detector Response:





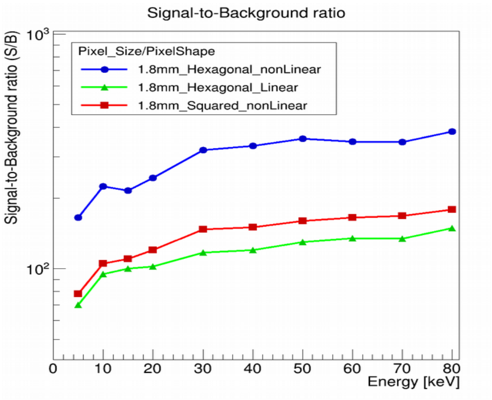


- Most of the events (84%) have cluster size equals 1, these events are collected in a single pixel.
- About 13% of the events are shared between two pixels (cluster size =2)
- Events with cluster size >=3 appears with low percentage (less than 2%).
- Pixel charge scan as a function of X @ y = 0.1 mm shows that the charge sharing region extension is measured to be 105 µm.

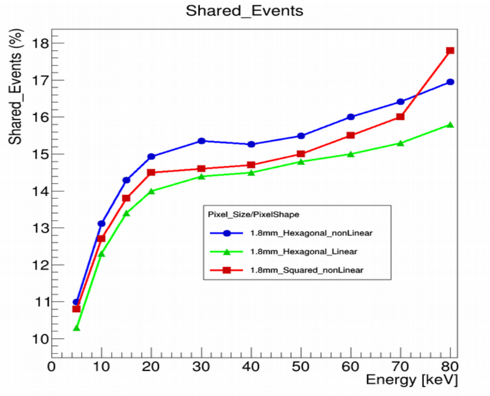
Hexagonal multi-element Ge detector

- Detector Response:

Allpix^2 – Non Linear Field



Allpix^2 – Non Linear Field



- The new hexagonal detector design shows a significant increase of the S/B at all energies.
- The new hexagonal pixel design shows a slightly higher percentage of shared events.
- These results show that hexagonal pixel design would be beneficial for future applications as it significantly increases S/B ratio and allows for a less extensive charge sharing in comparison with a conventional squared pixel design.

Summary

- New generation of multi-element germanium detectors for X-ray spectrometry is under development. However, detailed sensor simulations are presently lacking

- Allpix-squared is a well-suited framework to perform those simulations. Moreover, its modular nature allows for the rapid inclusion of new features.

- Contributed to develop customised version of allpix-squared that include:
    - New material, germanium, with its corresponding mobilities
    - New geometries: hexagonal pixel shape
    - Successfully used for studying variant designs of germanium detector. Preliminary results showed good agreement with experimental data.

- This work provide a reliable full simulation chain to simulate germanium detector with hexagonal pixel shape in different configuration for future applications.

- **Work in progress:**

    - Make the hexagonal allpix-squared extension described in this presentation accessible to the community

    - Include other high-Z materials commonly used in detectors for X-ray spectroscopy, e.g. CdTe

    - Include Pileup effects in simulation