PSI Center for Photon Science

Optimizing Charge Sharing Simulation

for Deep Learning Enhanced Spatial Resolution of the MÖNCH Detector

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Outline

Introduction

Optimizing simulation

Validation

Discussion and summary

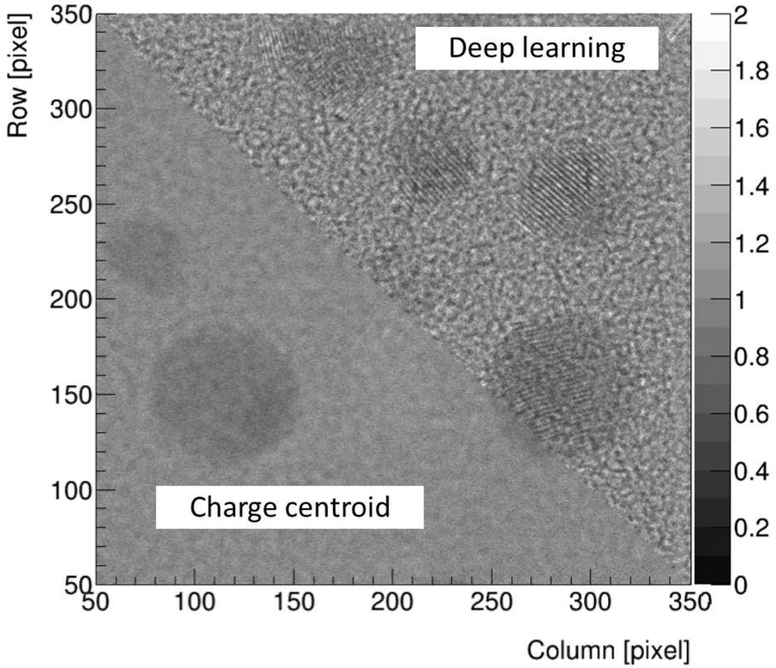
Introduction: Deep Learning Enhanced Spatial Resolution of the MÖNCH Detector

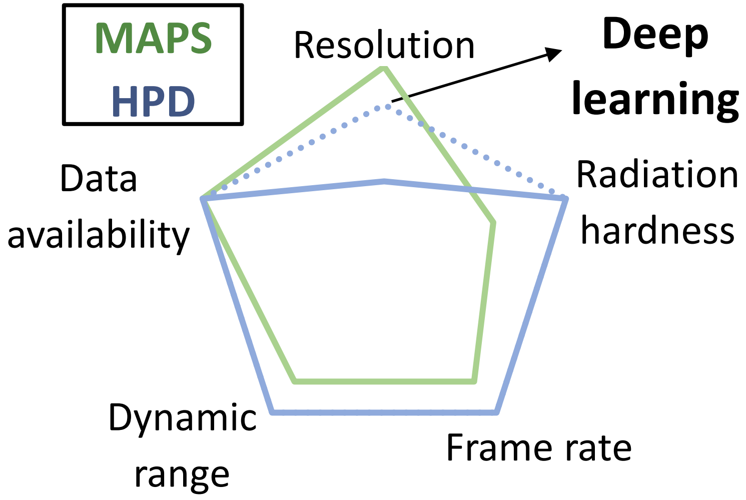
MÖNCH key specifications

- 25 um hybrid pixel detector with silicon sensor
- Charge integrating mode, 6 kHz frame rate

<u>Previous study</u>

- Use deep learning to reconstruct incident position of each 200 keV electron
  - To learn the nature of **electron multiple scattering** and **charge diffusion**
- Spatial resolution improved by **a factor of three** [1]
  - Experiment-based training: 0.60 pixel
  - Simulation-based training: 0.70 pixel
- Potential in electron microscopy applications





[1] X. Xie *et al* 2024 *JINST* **19** C01020

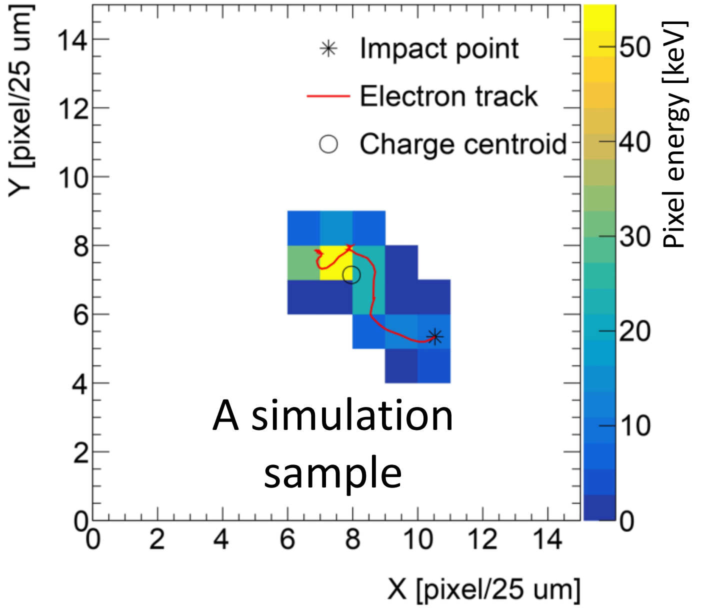
Introduction: Discrepancy between Simulation and Measurements

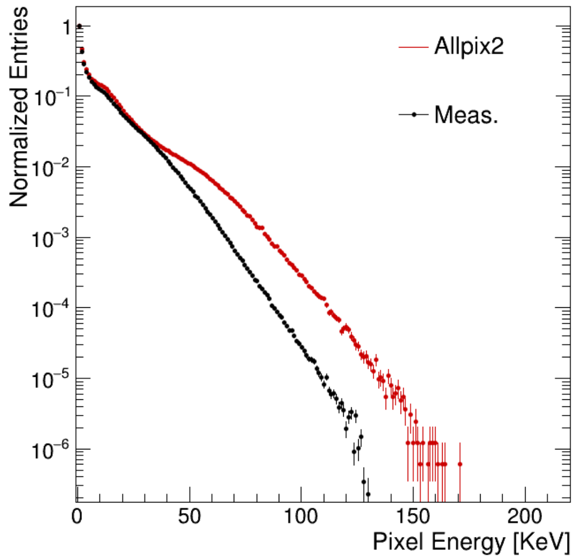
Simulation samples still matter

- Availability and flexibility
    - No special experimental setup required
    - Different electron energies
    - Different detector designs
- More information
    - 3D electron trajectory in silicon sensor

Single Pixel Energy Spectrum for electrons

- Pixels selected from 200 keV electron clusters
- Simulation tool: Allpix2
    - *Projection propagation module* to simulate drift and diffusion of charge carriers





Introduction: Discrepancy in Single Pixel Energy Spectrum for X-rays

Further investigation using X-ray

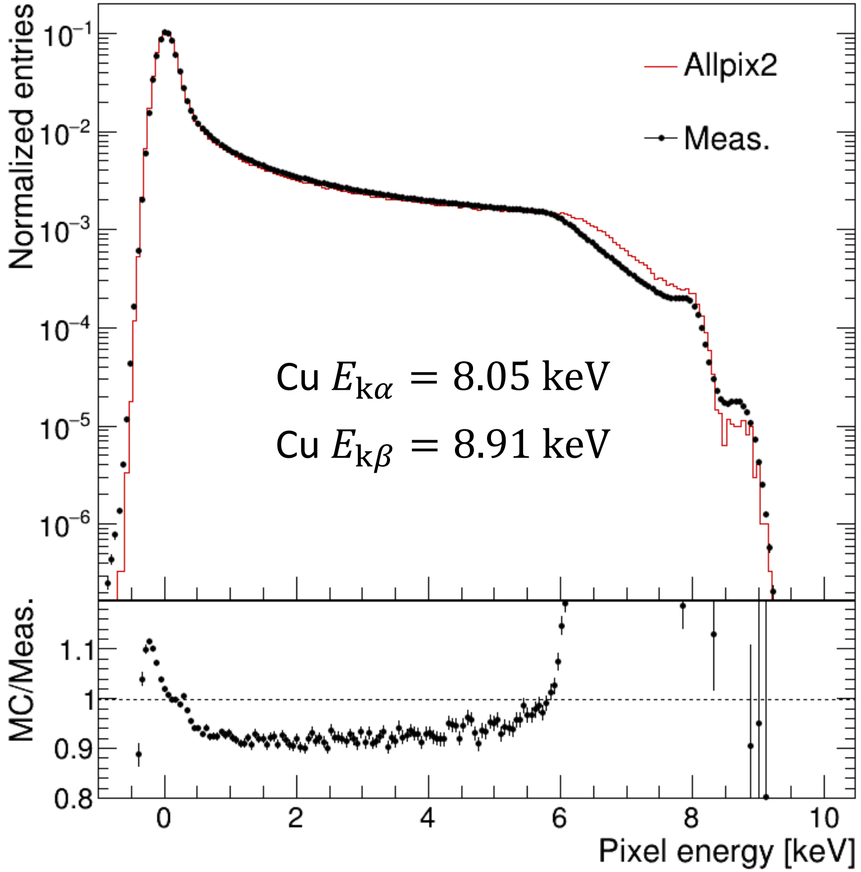
- Simplest case without particle trajectory
- Energy deposited in a point-like region

Pixels selected from 3x3-pixel clusters

- Same Allpix2 simulation setup
- Measured using X-ray tube

Discrepancy remains

- Simulation overestimates pixel energy
- Chare sharing is underestimated
- Discrepancy related to deposited energy



Reason: absence of repulsion simulation

Introduction: Charge Carrier Dynamics in Silicon

Continuity equation for charge carriers in silicon: $\frac{\partial p}{\partial t} = \underbrace{D\Delta p}_{\text{diffusion}} - \underbrace{\nabla \cdot (p\mu\vec{E})}_{\text{repulsion}}$

- $p(r, t)$: charge carrier density
- $D = \mu \frac{kT}{q}$, Einstein equation
- Drift treated independently

By neglecting the charge repulsion

- Simplified to be $\frac{\partial p}{\partial t} = D\Delta p$
- 1D solution $p(x, t) \sim N(0, \sqrt{2Dt})$
- Implemented in current allpix2 propagation modules

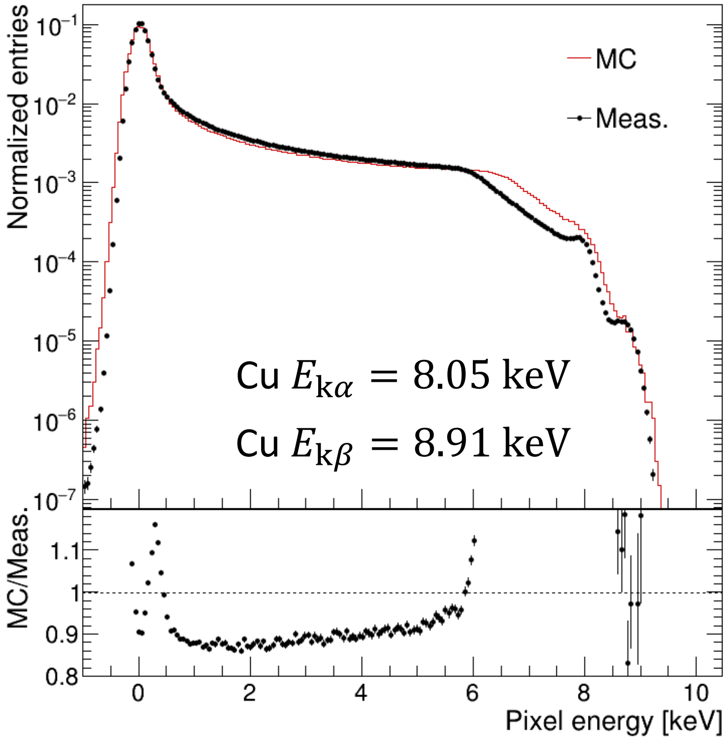
But not the case for HPD for X-ray/electron detection

- Deposited energy up to several dozen keV
- Charge repulsion is not negligible

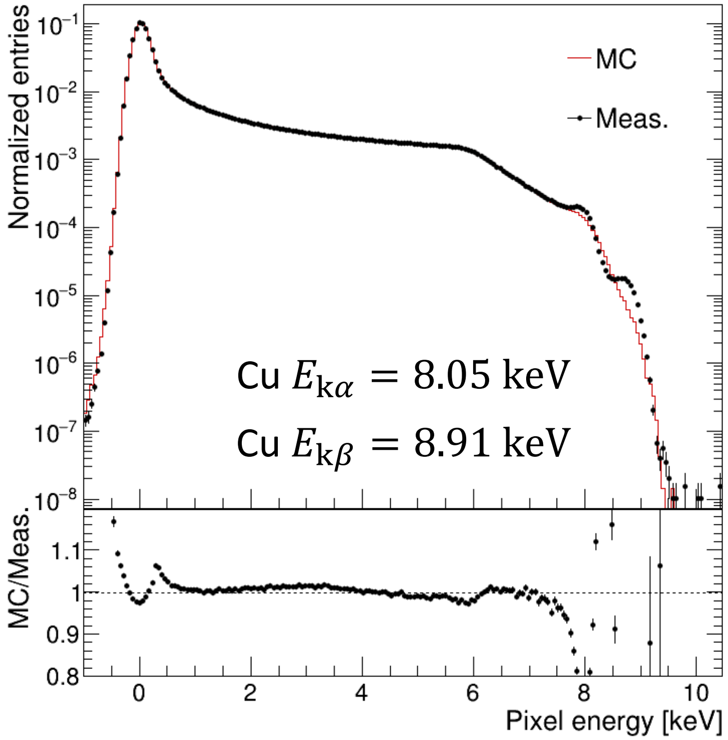
Introduction: Results of the Optimized Simulation

With repulsion simulated, more consistent Monte-Carlo simulation achieved

without repulsion



with repulsion



Optimizing Simulation: Recipe of Time-stepping MC Simulation

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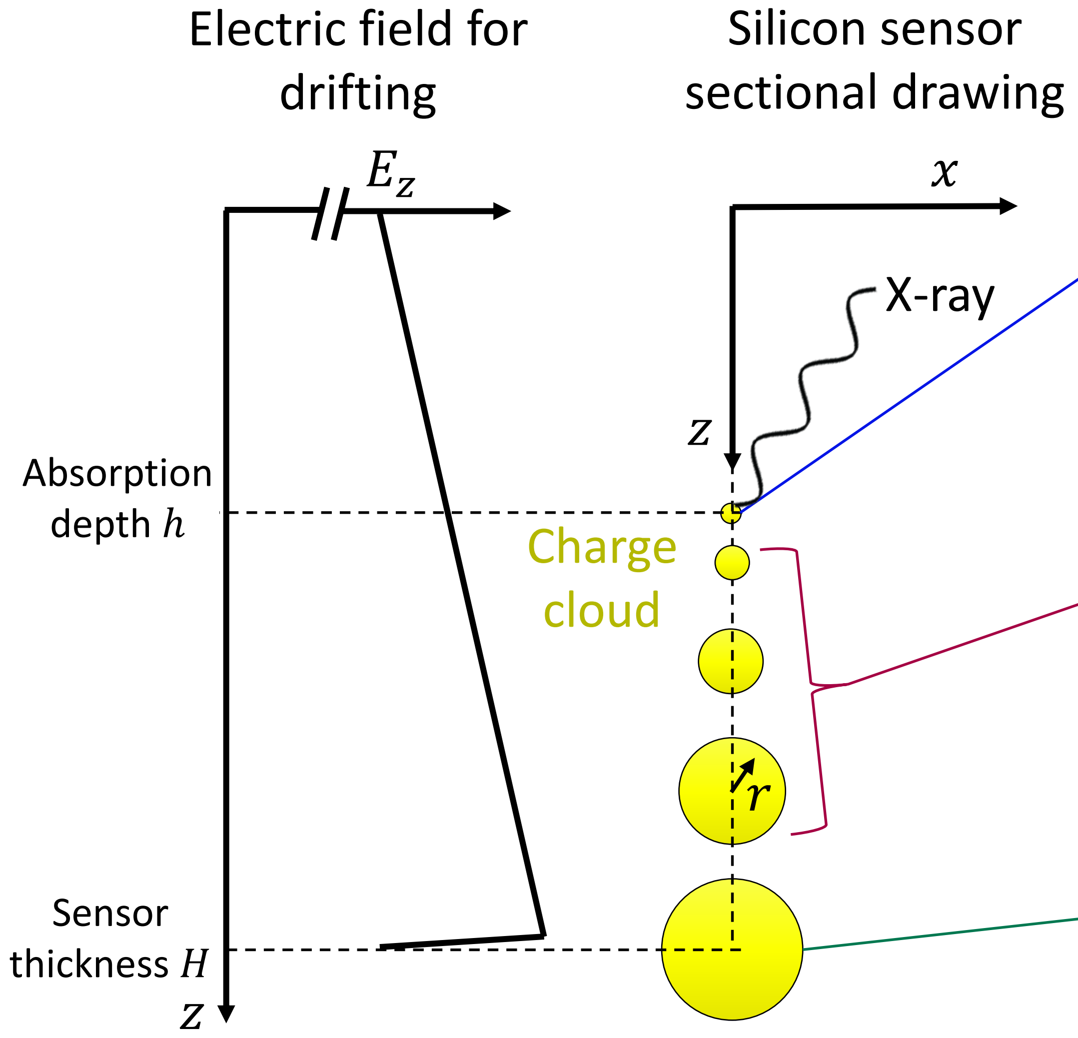


1. Photon absorption at $z = h$

- Empirical gaussian model for initial charge cloud: $\sigma = 0.0044 \cdot E^{1.75}$ µm [1]
- $\sigma = 0.17$ µm for 8.05 keV X-ray

2. Charge cloud drift

- Drift of cloud center: $z_{t+\delta t} = z_t + \mu E_z \delta t$

3. Propagation of a charge carrier at radius of r

- Diffusion: $r_{t+\delta t} = r_t \pm \sqrt{6D\delta t}$
- Repulsion: $r_{t+\delta t} = r_t + \mu E_r \delta t$
  - $E_r = \frac{Q(r)}{4\pi\epsilon r^2}, Q(r) = \sum_{r_i<r} q_i$

4. Simulation finished

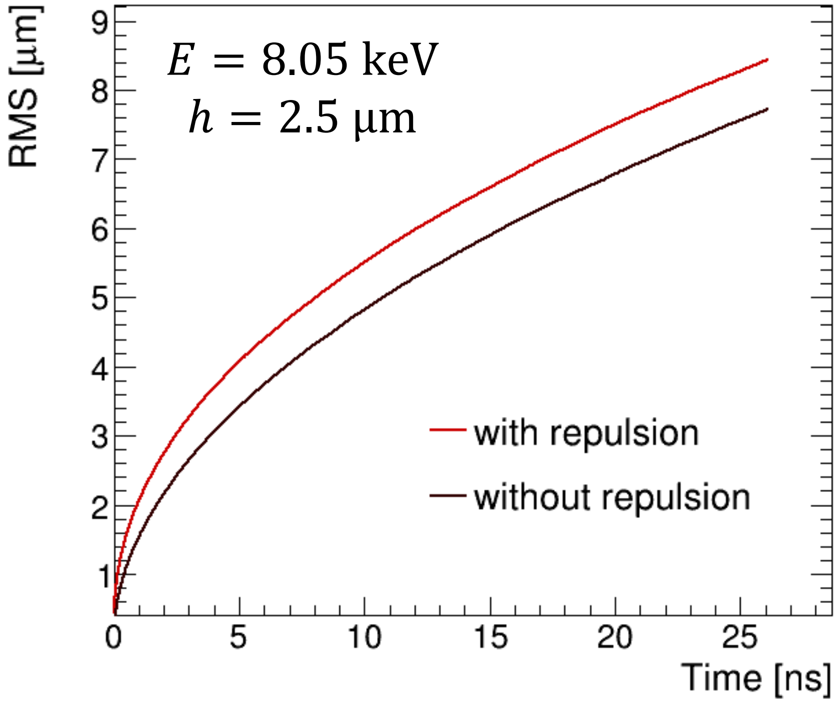
- When charge cloud center reaches sensor bottom $H = 320$ µm

[1] M.Lundqvist, Silicon strip detectors for scanned multi-slit X-ray imaging, Ph.D. Thesis, Royal Instituteof Technology(KTH), Stockholm, 2003.

Optimizing Simulation: Intermediate Results

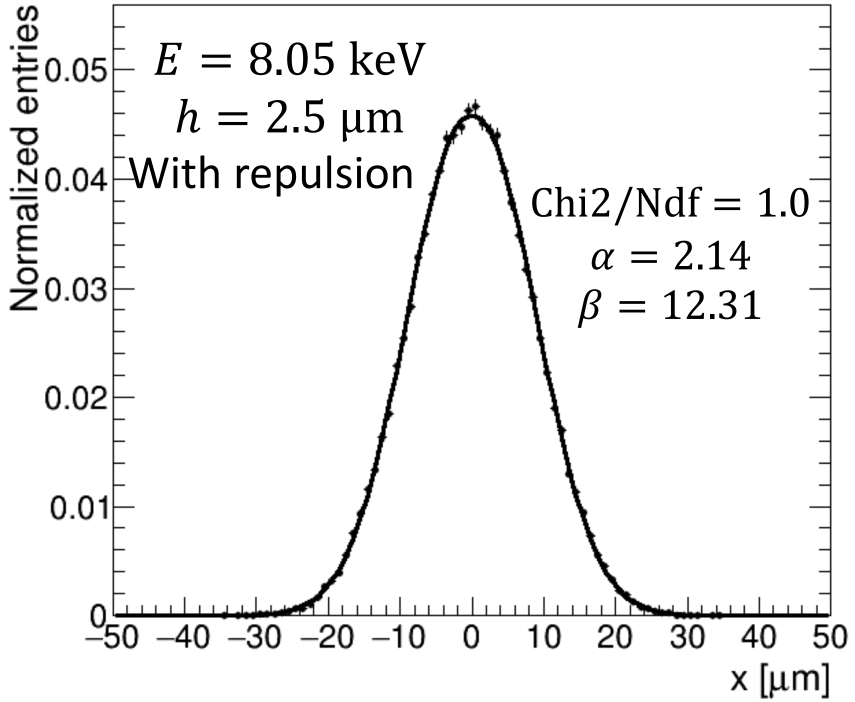
Example: absorption depth $h = 2.5\ \mu m$

- With repulsion, final RMS $= 8.46\ \mu m$
- Without repulsion, final RMS $= 7.68\ \mu m$



Charge carriers follow the generalized gaussian distribution (GGD)

$$p(x) \sim \frac{\beta}{2\alpha\Gamma\left(\frac{1}{\beta}\right)} \mathrm{Exp}(-|x|/\alpha)^{\beta}$$



Validation: Forming 3x3-pixel Cluster

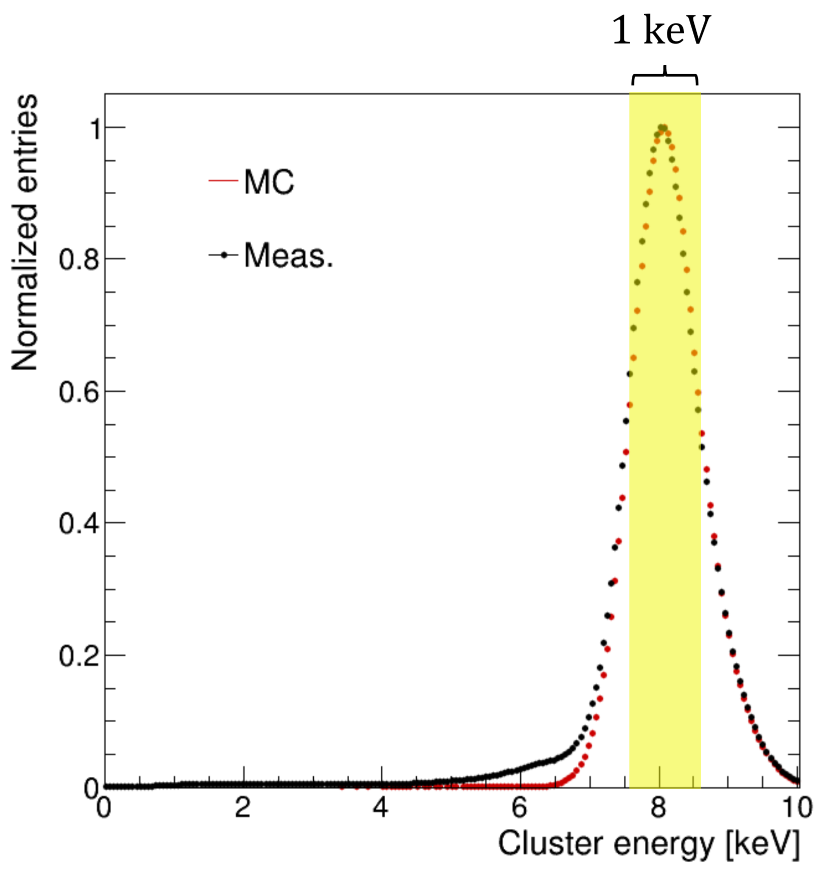
For simulation

1. Simulation conducted at different h every 5 μm
2. X-ray absorption depth h sampled from $\mathrm{Exp}(-\frac{h}{\lambda})$
3. Charge carriers x, y sampled from $\mathrm{GGD}(\alpha, \beta)$
4. Add noise (~ 0.13 keV) and form a 3x3-pixel cluster

For measurement

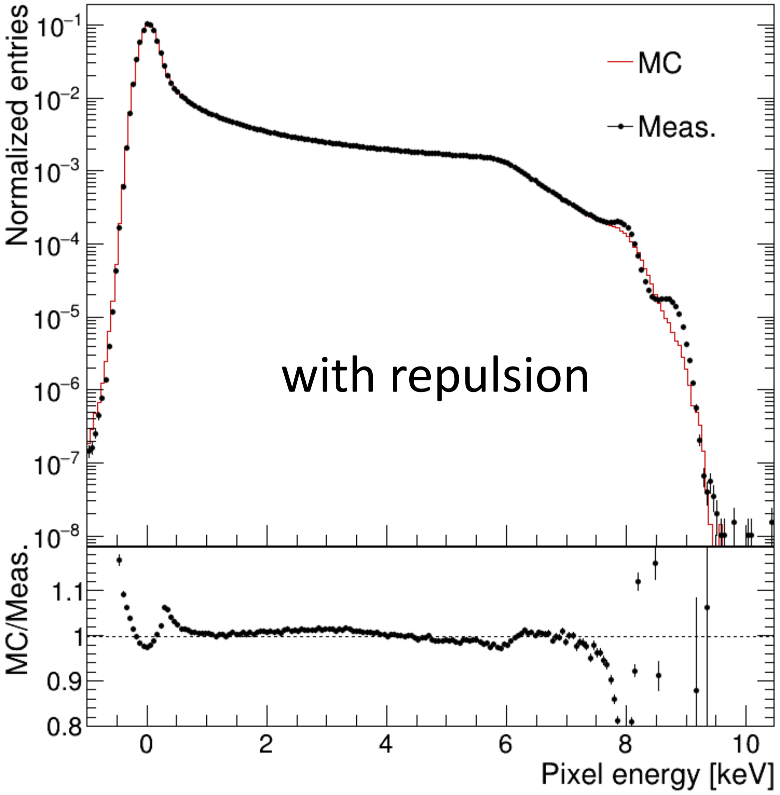
- Pedestal subtracted
- Pixel-wise gain calibration applied
- Cluster finding

Cluster energy window: $(E_{\mathrm{k}_\alpha} - 0.5\ \mathrm{keV}, E_{\mathrm{k}_\alpha} + 0.5\ \mathrm{keV})$

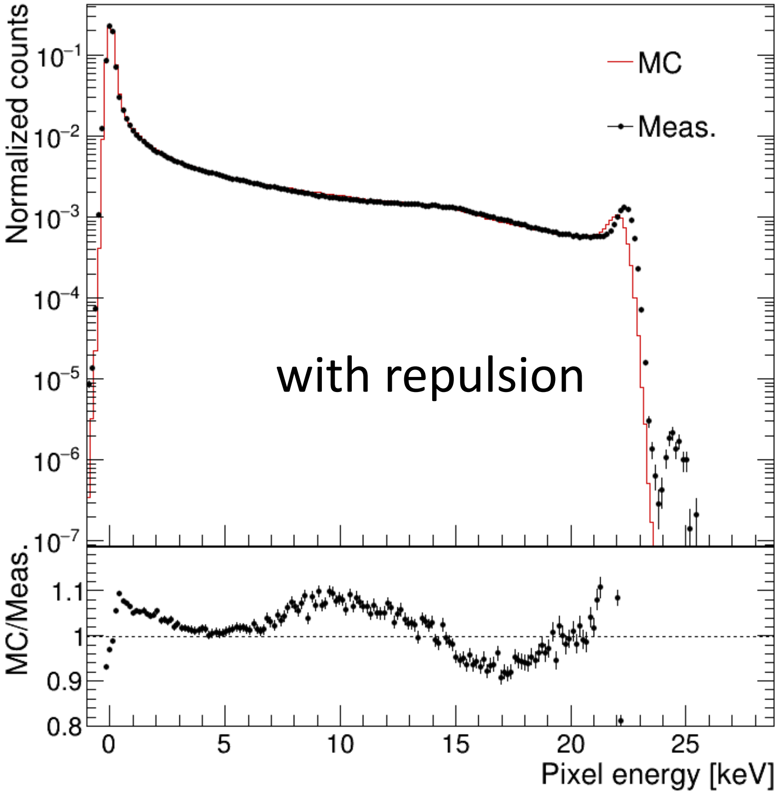


Validation: Pixel Energy Spectrum

Cu $E_{k\alpha} = 8.05\ \mathrm{keV}$
Cu $E_{k\beta} = 8.91\ \mathrm{keV}$

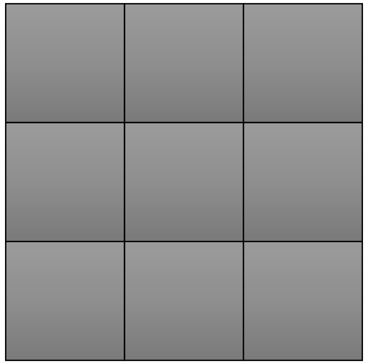


Ag $E_{k\alpha} = 22.16\ \mathrm{keV}$
Ag $E_{k\beta} = 24.94\ \mathrm{keV}$



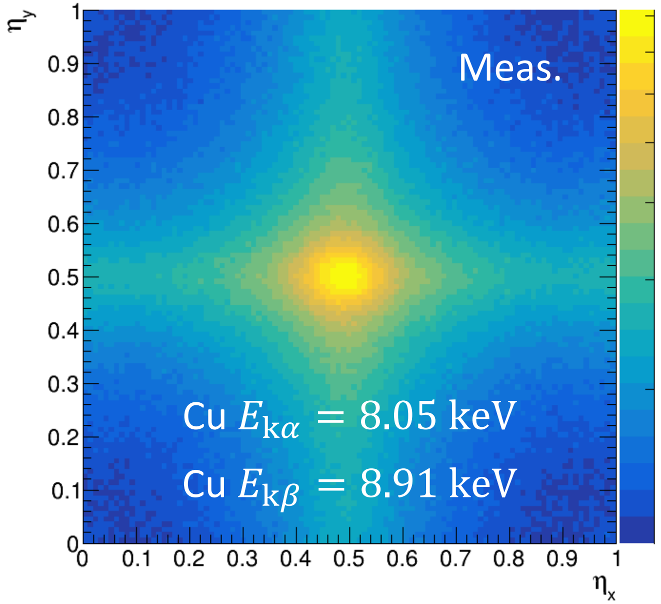
Validation: Charge Weighted Center η_x, η_y

3x3-pixel cluster

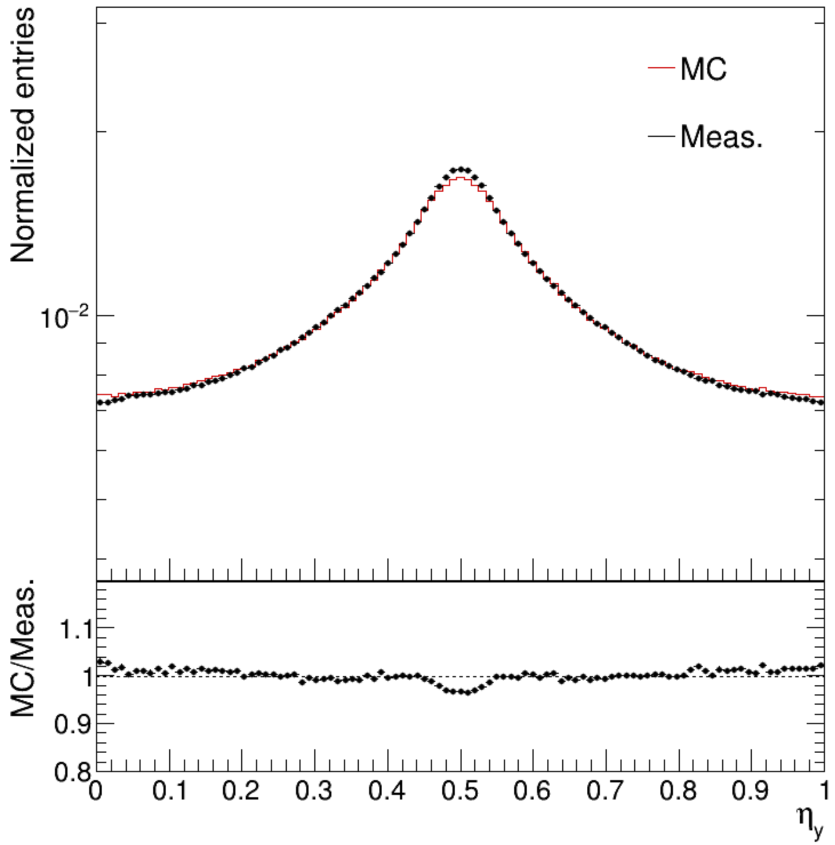


$$\eta_x = \frac{\Sigma_i Q_i \cdot x_i}{\Sigma_i Q_i} \text{ [1]}$$

$$\eta_y = \frac{\Sigma_i Q_i \cdot y_i}{\Sigma_i Q_i}$$



Projection



[1] E. Belau, et al. (1983). *Nucl. Instrum. Methods Phys. Res*. **214**, 253–260.

Discussion

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Source of remaining mismatch

- Spherical symmetry assumption for charge cloud
  - Gradient of E_z inside charge cloud ignored
  - Asymmetry ignored when charge cloud approaching sensor bottom
- Uncertainty in measurements and modeling
  - Mobility μ, noise modeling
  - Gain uncertainty and non-linearity
  - Pixel crosstalk

To implement for electron simulation

- Parameterization of α, β as functions of absorption depth and E_{deposit}
- Repulsion between adjacent charge clouds

Summary

Charge sharing simulation has been optimized

- Repulsion simulation should be considered for small pixel HPD for X-rays/electrons
- Good agreements obtained between measurements and the proposed simulation

To implement as an Allpix2 module

- Better quality of simulation samples for deep learning
- Help optimize detector design by exploiting charge sharing

Thank You!

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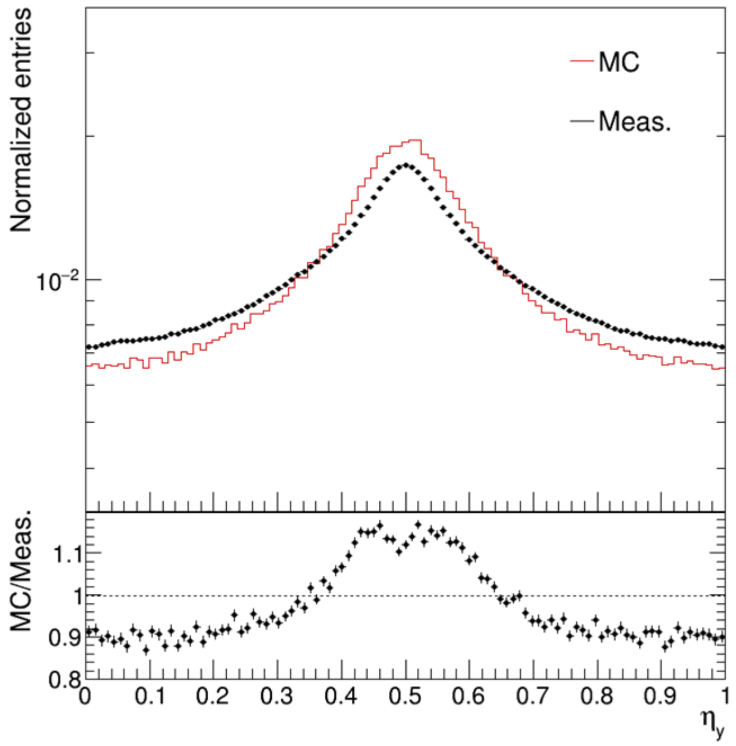
Jiaguo, Victoria, Shqipe, Anna, Xiangyu, Roberto, Bernd
Missing: Erik, Aldo, Rebecca, Simon, Davide, Dhanya

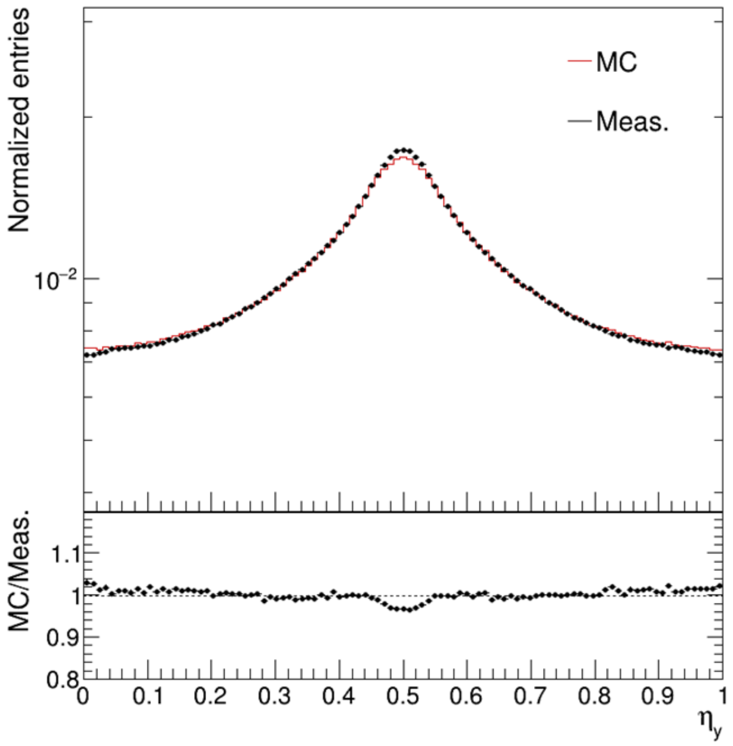
Backup Validation: Charge Weighted Center η_y

Cu $E_{k\alpha} = 8.05$ keV
Cu $E_{k\beta} = 8.91$ keV

without repulsion



with repulsion



Backup Optimizing Simulation: Preparations

Coordinates system conventions

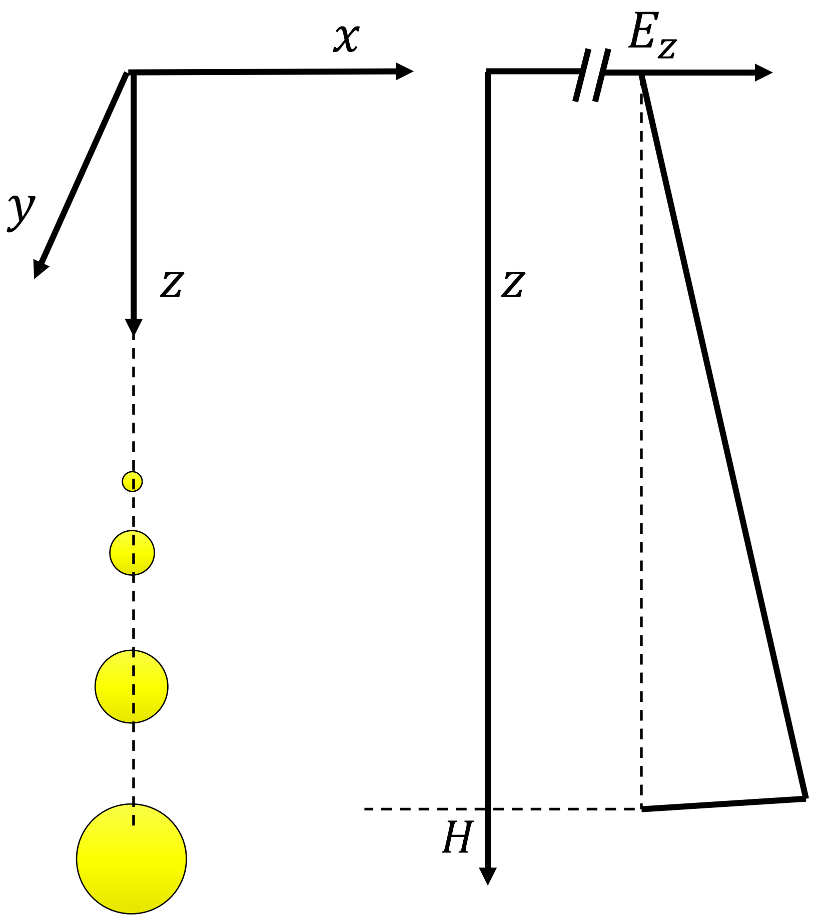
- xy plane is the sensor plane; z axis points backward
- Charge center $(0, 0, z_{\text{center}})$ drifts from $(0, 0, h)$ to $(0, 0, H)$
  - Absorption depth h; sensor thickness $H = 320\ \mu\text{m}$

Drifting electrical field

- $E_z(z) = \frac{V_{\text{bias}} - V_{\text{dep}}}{H} + \frac{2V_{\text{dep}}}{H} \cdot \frac{z}{H}$
- $V_{\text{dep}} = 30\ \text{V}, V_{\text{bias}} = 90\ \text{V}$

Initial charge cloud distribution

- $\sigma = 0.0044 \cdot E_{\text{deposit}}^{1.75}\ \mu\text{m},$
- Jacoboni-Canali mobility model
- $\mu(E) = \frac{v_m}{E_c} \frac{1}{\left(1 + (E/E_c)^{\beta}\right)^{1/\beta}}$



Backup Optimizing Simulation: Recipe of Time Stepping Monte Carlo Simulation

Dynamics of a charge carrier at $(x, y, z + z_{\text{center}})$ while the charge center at $(0, 0, z_{\text{center}})$

- $\boldsymbol{E}(x, y, z + z_0) = \boldsymbol{E}_{\textbf{repulsion}} + \boldsymbol{E}_{\textbf{drift}}$
  - $\boldsymbol{E}_{\textbf{repulsion}}(x, y, z + z_0) = \frac{Q(r)}{4\pi\epsilon r^2}(\frac{x}{r}\boldsymbol{e_x} + \frac{y}{r}\boldsymbol{e_y} + \frac{z}{r}\boldsymbol{e_z})$
    - $Q(r) = \sum_{i \text{ where } \sqrt{x_i^2+y_i^2+z_i^2}<r} q_i$
    - Hold under the assumption of spherical symmetry of charge cloud
  - $\boldsymbol{E}_{\textbf{drift}}(z + z_{\text{center}}) \cong \boldsymbol{E}_{\textbf{drift}}(z_{\text{center}}) = \left(\frac{V_{\text{bias}} - V_{\text{dep}}}{H} + \frac{2V_{\text{dep}}}{H}\frac{z_{\text{center}}}{H}\right)\boldsymbol{e_z}$

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

Coordinates updating for each charge carrier

- Repulsion: $x[t + \delta t] = x[t] + \mu(|\boldsymbol{E}|)|\boldsymbol{E}|\frac{x}{\sqrt{x^2+y^2+z^2}}\delta t$, $\delta t \coloneqq 0.01 \text{ ns}$
- Diffusion: $x[t + \delta t] = x[t] \pm \sqrt{2D\delta t}$, $D = \mu(|\boldsymbol{E}|)\frac{kT}{q}$ modelled as random walk