SKADI instrument simulation

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My (relevant) background

- PhD (2017-2021): *Full Simulation of Detector Performance of Neutron Instrumentation at ESS*
  - **McStas** (from the neutron source to the sample) + **Geant4**: (detector system)
  - Geant4 simulation study of the BCS detectors (used for LOKI)
  - Estimate the expected intensities for LOKI (and for BIFROST)

- Geant4 simulation model of the complete LOKI detector assembly
  - Generating simulated data to support the creation/testing of calibration and data reduction routines
  - Got involved in the creation of the NeXus/JSON geometry file

- Now: SKADI detector simulation model

SKADI detector simulation plan

- Main task: implement a simulation model of the full SKADI detector system with representative detector geometry instead of simple McStas monitors

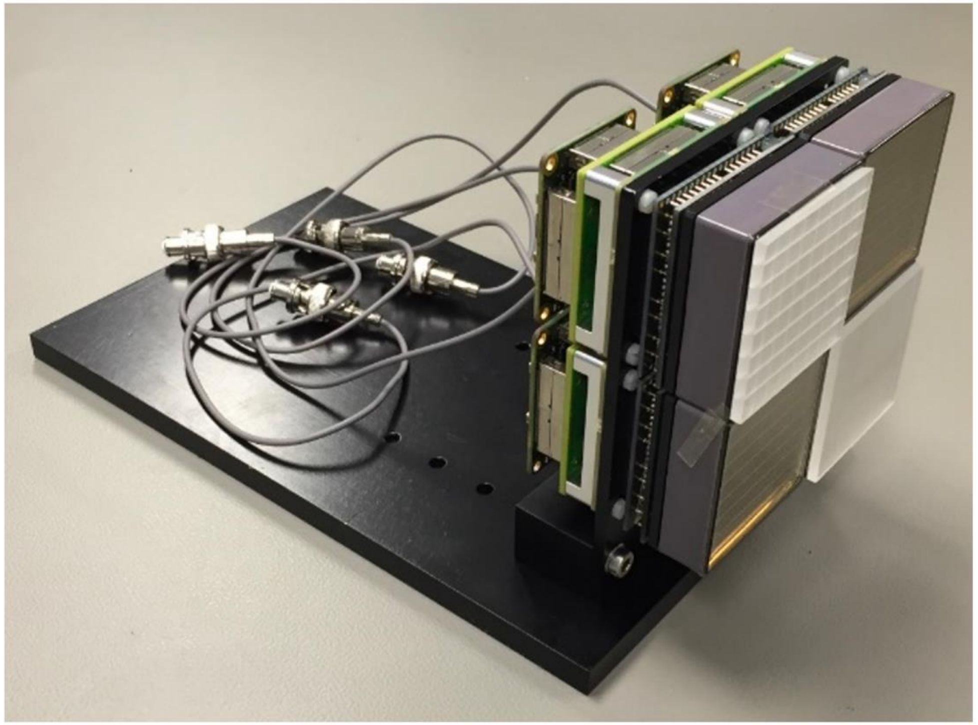
- Modelling SoNDe with McStas (UNION+NCrystal)
  - Implement the SoNDe detector geometry with UNION components
  - Simulate neutron transport and absorption(ideally in the GS20 converter layer)
  - Use representative detector response function to get detection from neutron absorption, based on Geant4 simulations (*function(...,w, x, y, z) → (w_det, pix_id)*)
    - Input: weight and x, y, z position of the neutron absorption in the GS20
    - Output: probability of detection events in SoNDe pixels
  - Output detection events in Nexus format compatible with Scipp processing

- Implement full SKADI detector system (extending the SKADI McStas model)

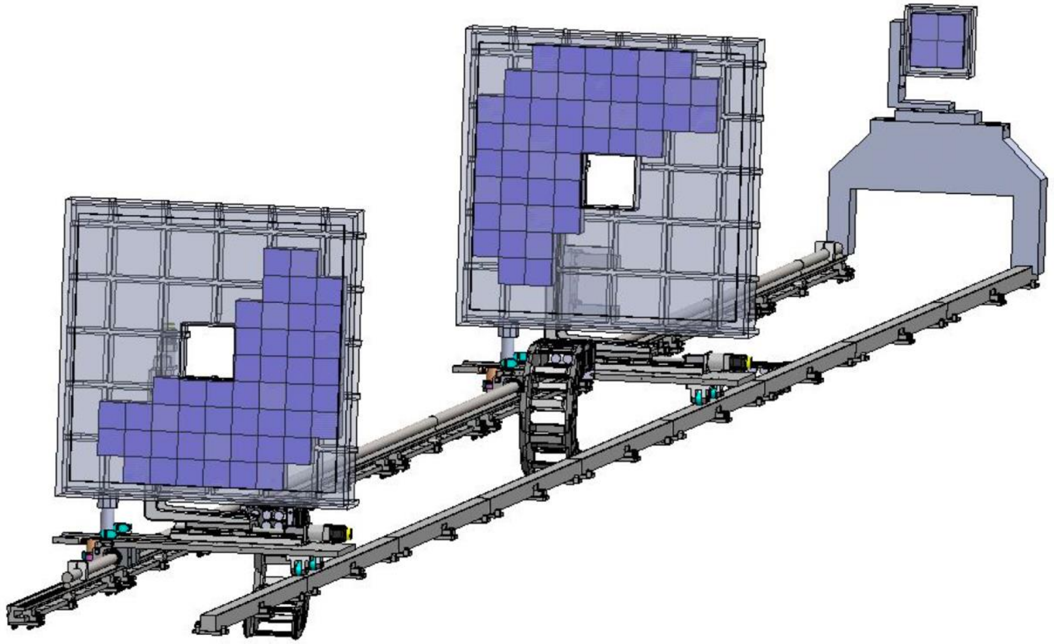
Outline

- **SoNDe Geant4 simulation**
- McStas model implementation
- The challenge on the non-uniform pixel sizes
- The challenge of the pixel ids
- Planned usages

SKADI detector system



(a)

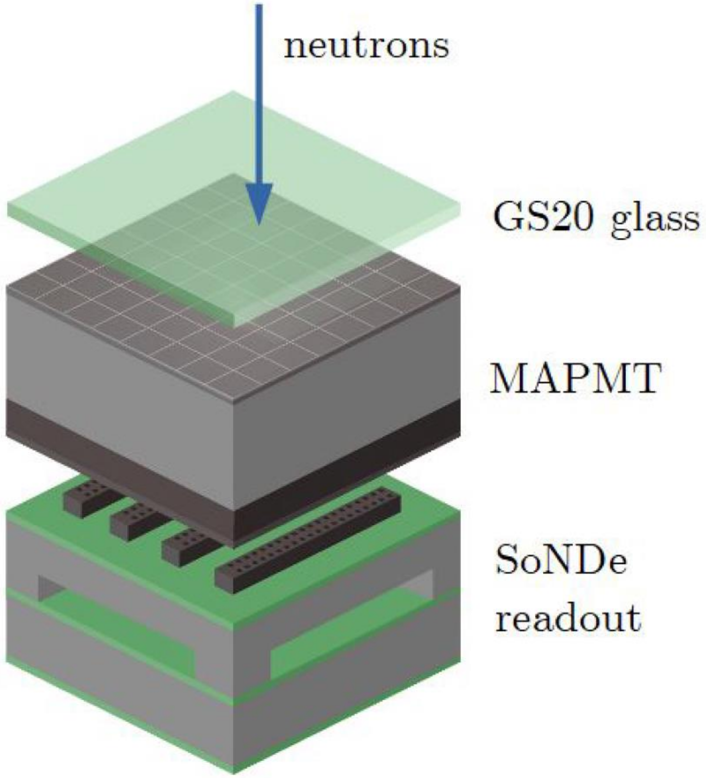


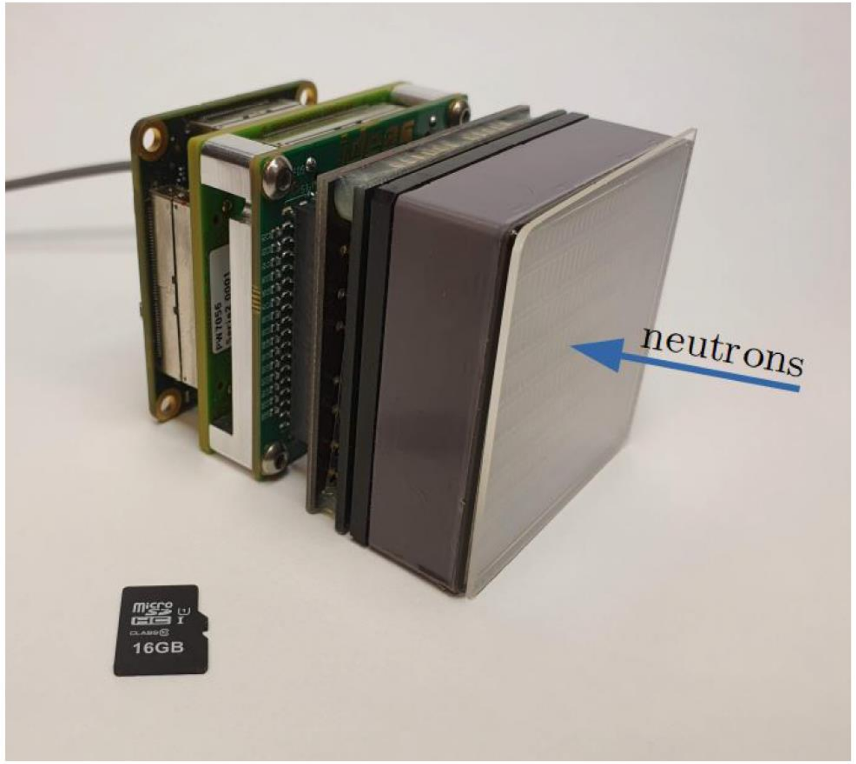
(b)

Figure 9. (a) Photograph of a 2x2 module of a SoNDe type detector. 2x2 module is ~10x10 cm in size. (b) Arrangement of active area tiles, as shown in (a) for the complete detector setup.

- Front/middle banks: 384 detectors (per bank) with 8x8 pixels
- Rear bank: 16 detectors with 16x16 pixels (high-resolution detectors)

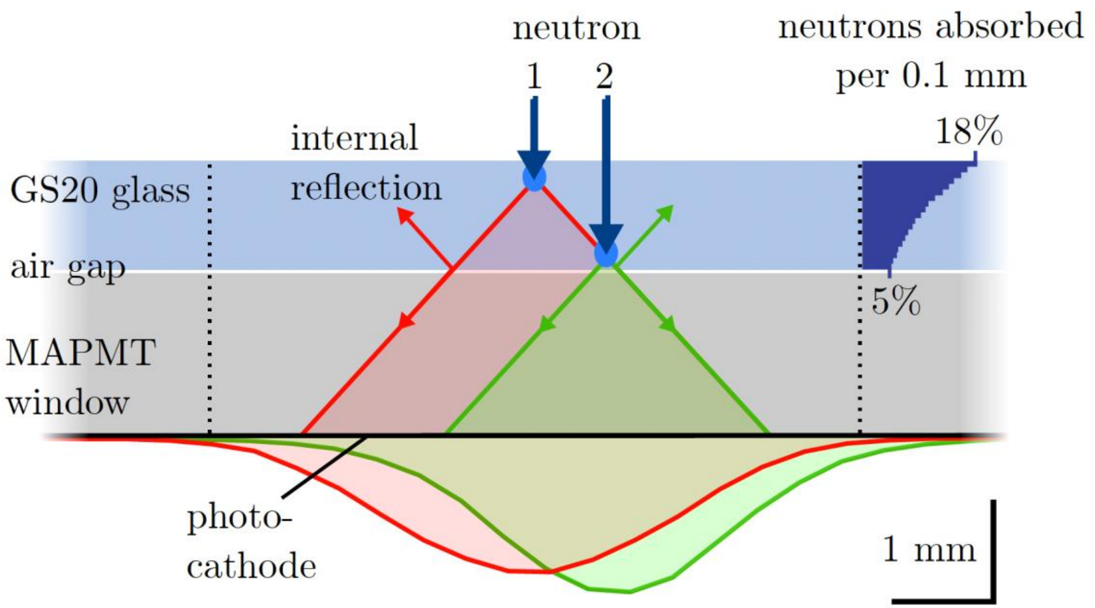
SoNDe –Solid-State Neutron Detector



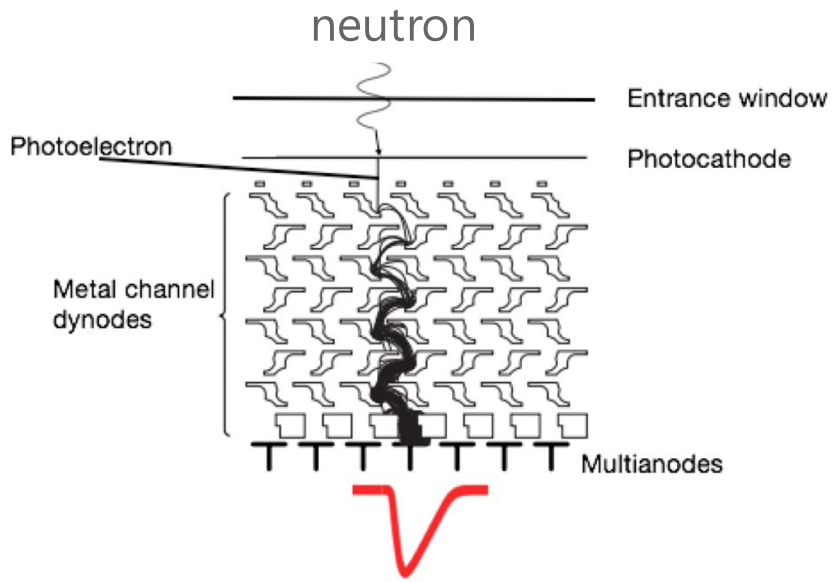


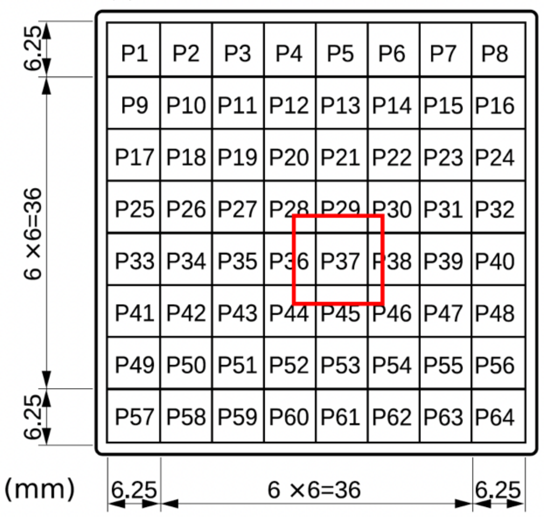
- 1 mm thick cerium-activated ^{6}Li glass scintillator sheet (GS20)
- 8 X 8 (64 pixel) multianode photomultiplier tube (MAPMT) (Hamamatsu model H12700A)
- Purpose-built readout electronics

Scintillation-light distribution / MAPMT



Scintillation-light distributions from GEANT4 . 2D representations of GEANT4 simulated scintillation-light cones (triangles) and photocathode yields (inverted normal distributions) resulting from interactions at the upstream GS20 surface (neutron 1, red) and the downstream GS20 surface (neutron 2, green). Vertical dotted lines indicate pixel edges. The number of interacting neutrons is shown as a function of penetration depth into the GS20 sheet in the top-right corner.





(b) MAPMT pixel map

- **Issue 1) Multiplicity**
  Scintillation light can spread to multiple pixels

- **Issue 2) Electronic crosstalk** Scintillation photons reaching the photocathode in one pixel can induce a signal in neighbouring pixels.

Multiplicity depending on threshold

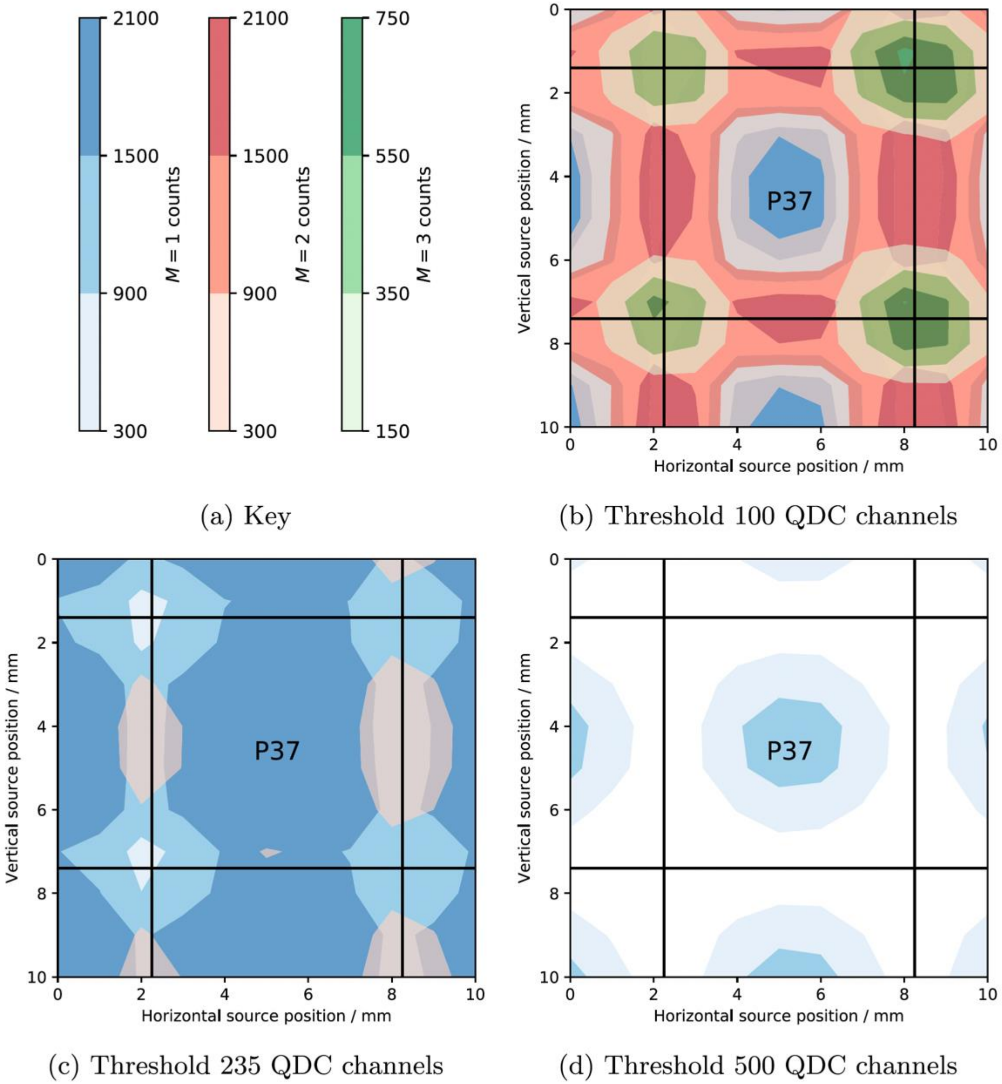
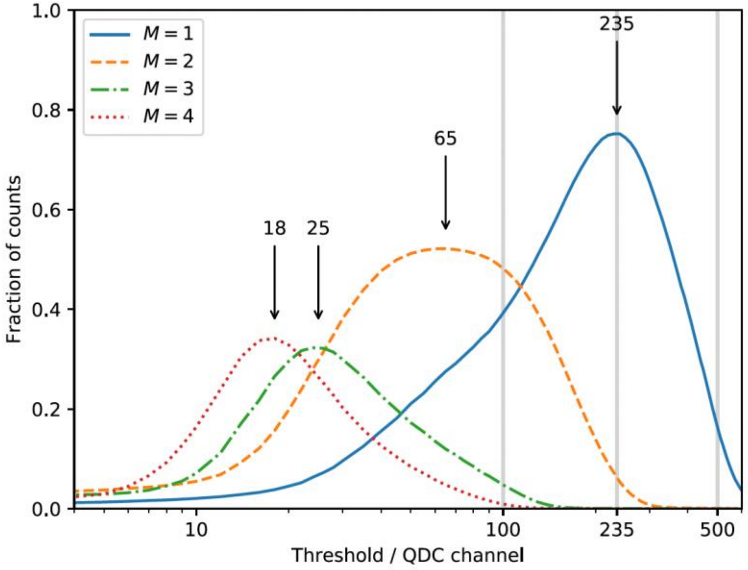


Fig. 6. Contour plots of the multiplicity distributions for pixels lying near P37 for different thresholds as a function of α-particle beam irradiation location. The black lines denote the pixel boundaries. In all three contour plots, blues indicate $M = 1$ events, reds indicate $M = 2$ events, and greens indicate $M = 3$ events. The lighter the shade of the color, the fewer the counts. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



(b) Practical multiplicities

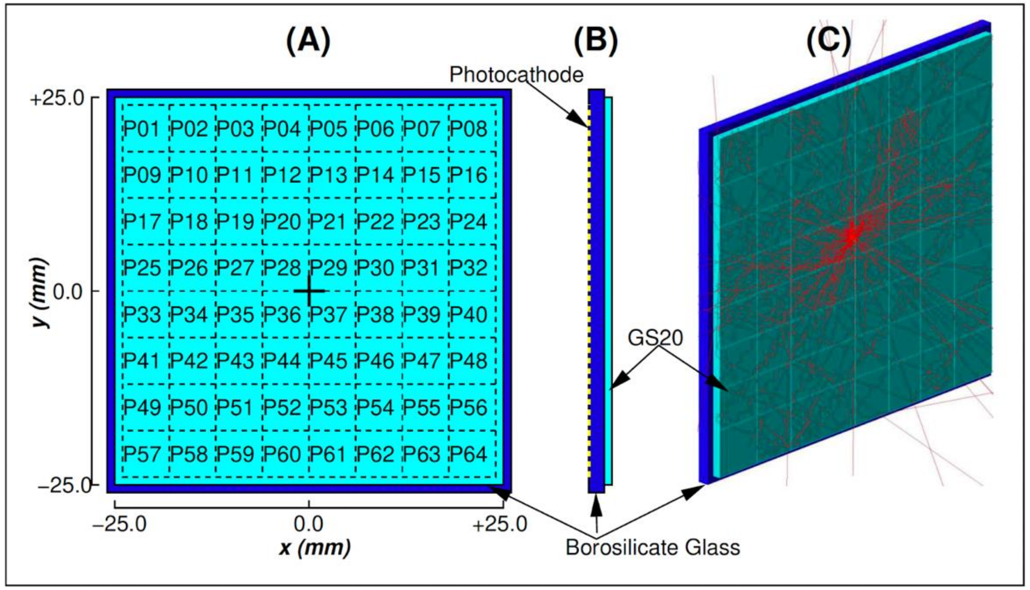
Fig. 7. Tuning the analysis using a single QDC threshold. Relationships between the relative number of events and threshold. Top Panel: $M = 0$ (black dot–dot-dashed line) and $M > 4$ (light blue dot-dashed line). Bottom Panel: $M = 1$ (dark blue solid line), $M = 2$ (orange dashed line), $M = 3$ (green dot-dashed line), and $M = 4$ (red dotted line). The gray vertical lines at QDC channel 100, 235, and 500 represent three of the QDC threshold cuts employed in Fig. 6. Arrows indicate the optimal values for QDC threshold cuts for tuning the resulting data set for a specific value of M. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

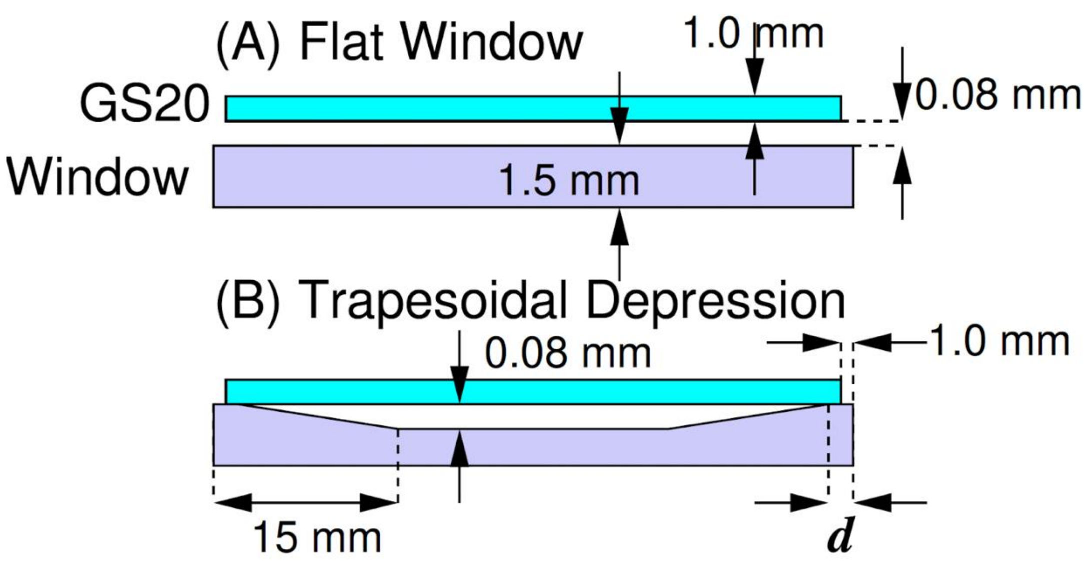
- **Intended usage is M=1** (due to DAQ limitations)

Geant4 simulation

- Using Geant4 model implemented by John Annand / Emil Rofors / Glasgow ppl
  Repo: https://git.esss.dk/milan.klausz/sonde_geant4

- Simulation of transport of neutrons, secondary particles, generation of scintillation photons, transport of these optical photons, and their "detection" on the photocathode (with energy dependent quantum efficiency)
- Analysis: for each neutron → counting "detected" photons in the photocathode area corresponding to each pixel (+ approximate electronic cross-talk), with detection threshold





Geant4 simulation – detection threshold

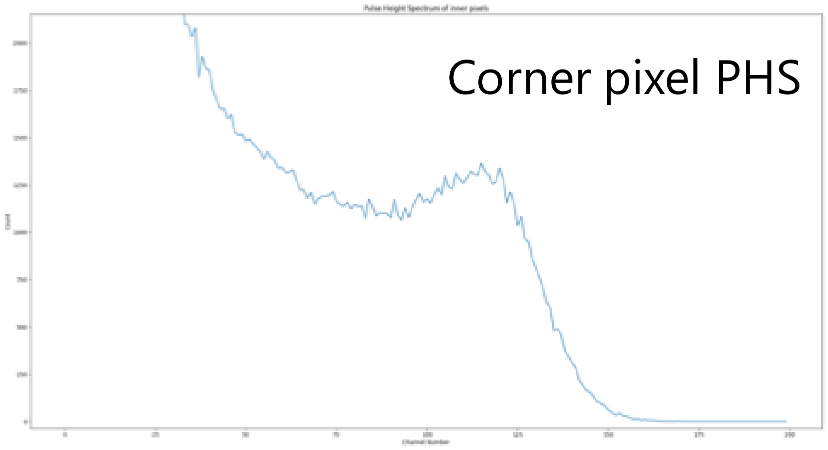
- Based on info from Ralf, the detection threshold is determined based on the pulse-heigh spectra of the pixels

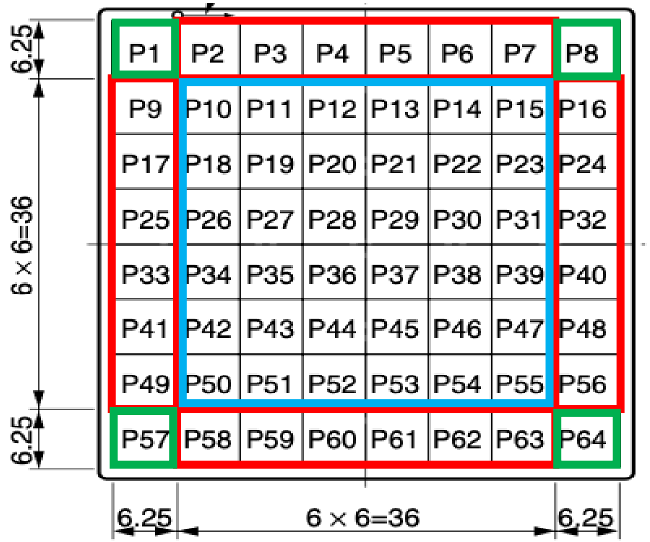
- The 3 different sized pixels need different values
  - **Corner pixels** / **Edge pixels** / **Inner pixels**

- Carried out a study with different illumination (pencil beam, uniform, uniform over illumination) of the different pixels

- Defined 3 thresholds (for the sum weight of the detected photons)

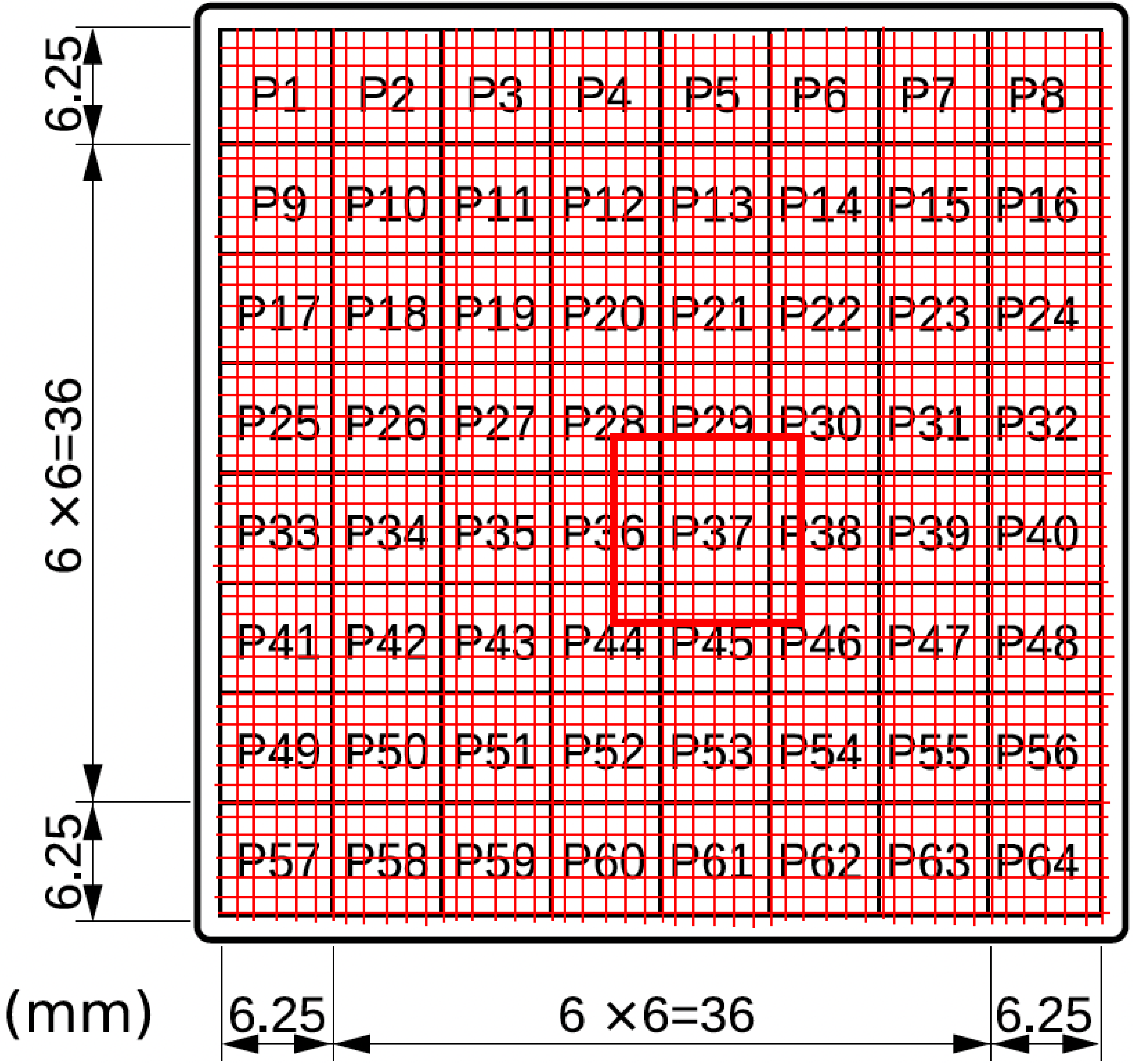
- **M>1 (single neutron, multiple pixel detection) events are negligible ~0.01% (as expected by Ralf)**



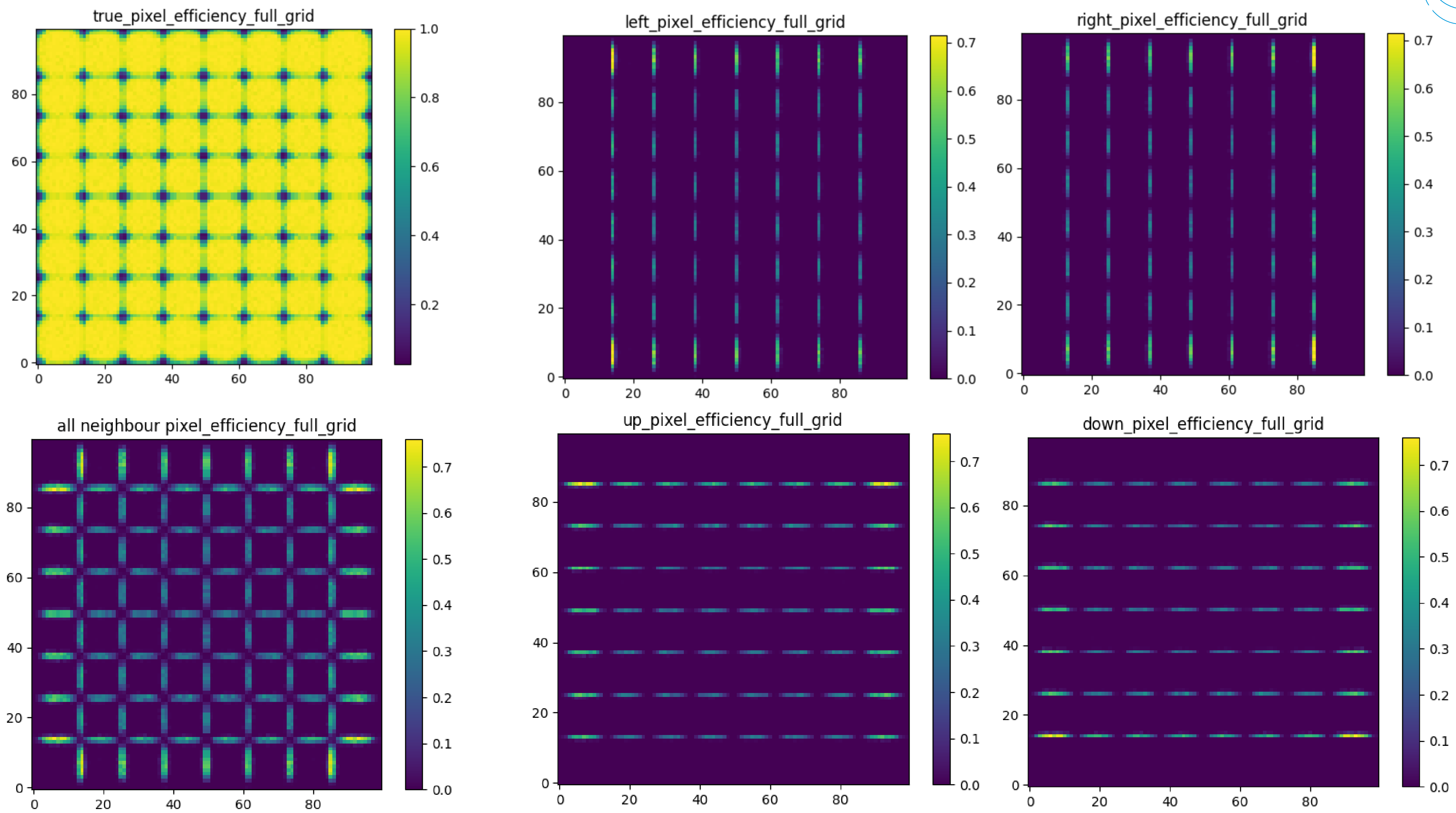


Geant4 simulation output

- 0.5x0.5 mm grid for neutron conversion position
- For each grid position: if a neutron is absorbed there, what is the probability of triggering a detection event
  1. in the pixel behind the grid position
  2. in the pixel to the left
  3. in the pixel to the right
  4. in the pixel to the top
  5. in the pixel to the bottom
- 5 numbers for each grid position
- Data arranged into 5 tables: true/left/right/up/down detection probability for each grid position



Geant4 simulation output (old result!!)



Geant4 simulation limitations/issues

- Each pixel should have different gain – which is corrected, so it is fine that it is not simulated)

- Position sensitivity within each pixel:
  - due to light share among pixels (simulated)
  - centre of each pixel is more sensitive due to the MAPMT geometry (NOT simulated)
    - This should lower the number of false detections (detected in a neighbouring pixel)

- The detection threshold is set manually, quite arbitrarily

- Simple detector model
  - Only the essential materials are included in the model
  - A single detector is simulated (no scattering effects)
  - Electronics (MAPMP) not modelled

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- SoNDe Geant4 simulation
- **McStas model implementation**
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McStas simulation model

- Using Union in McStas to allow scattering among multiple components
- Using NCrystal materials: GS20 converter layer, Borosilicate MAPMT window

- Needed a ”monitor” component that I can tamper with
- **Union_abs_logger_nD_scintillator.comp**
  - Based on the *Union_abs_logger_nD component* from Mads Bertelsen
  - Reads the tabular detection efficiency data (~csv files) from Geant4
  - When a neutron is absorbed in the GS20 layer, its Monte Carlo weight is multiplied with detection efficiency from the table (based on x,y coordinate)
  - Adding multiple detection events to the nD monitor in case of non-zero chance of detection in neighbouring 4 pixels (very low chance)

  - Due to the uniform bin size of the *monitor_nD*, 6 mm pixels are used, but detection events on the outer perimeter of the detector (0.25mm) are moved inside the pixel by 0.25mm
    - This will be explained in detail later…

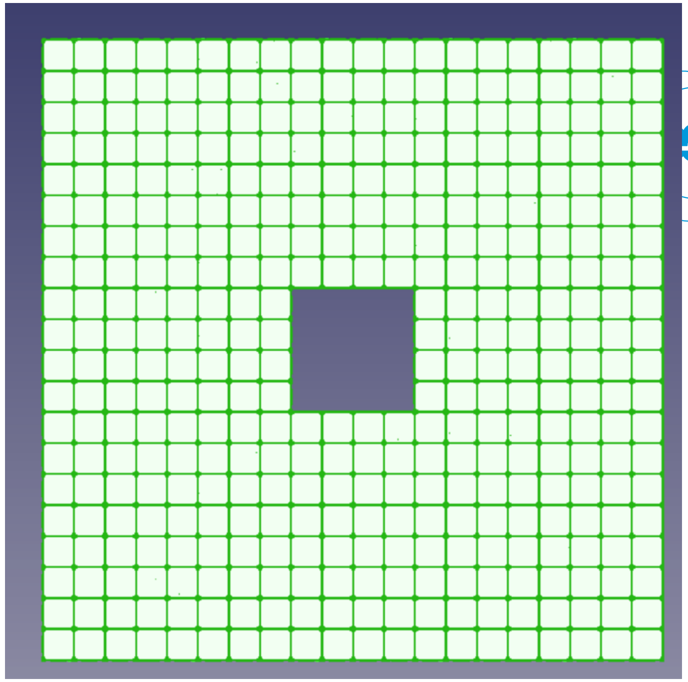
McStas simulation model

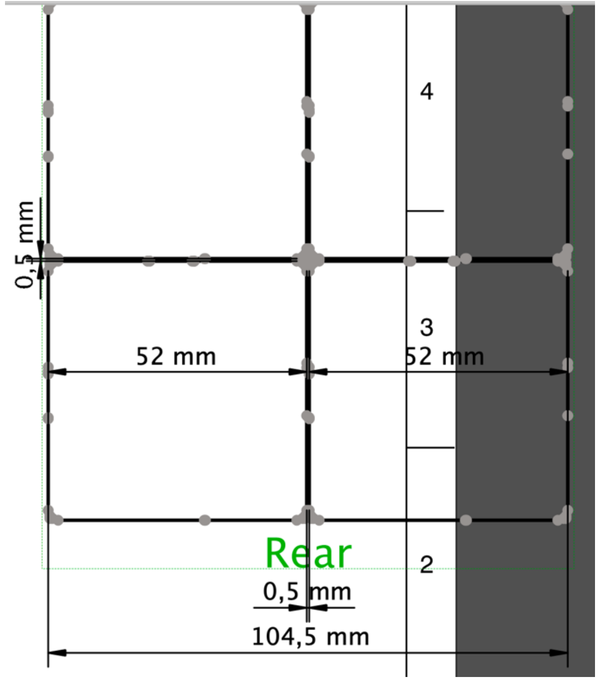
- Single SoNDe detector module model:
  - GS20: *Union_box* with NCrystal material
  - MAPMT_Window: *Union_box* with NCrystal material
  - *Union_abs_logger_nD_scintillator*

- Need to position 784 detectors → using McStasScript

Detector geometry

- Detector positioning:
  - Building block: 2x2 detector tiles
  - Positions based numbers extracted from CAD file
  - Very symmetric!
- Space between detectors in a tile: 0.5 mm
  - This is the same distance between the tiles
- Note: 52 mm detector size vs sum pixel size of 48.5 mm (sensitive area)
- Rear bank high-resolution detectors has the same physical dimensions, but 16x16 pixels (instead of 8x8)



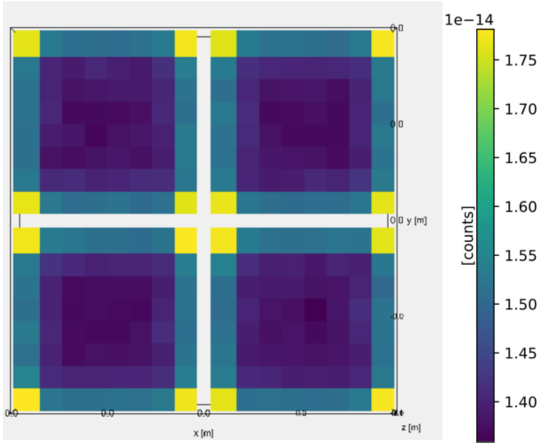


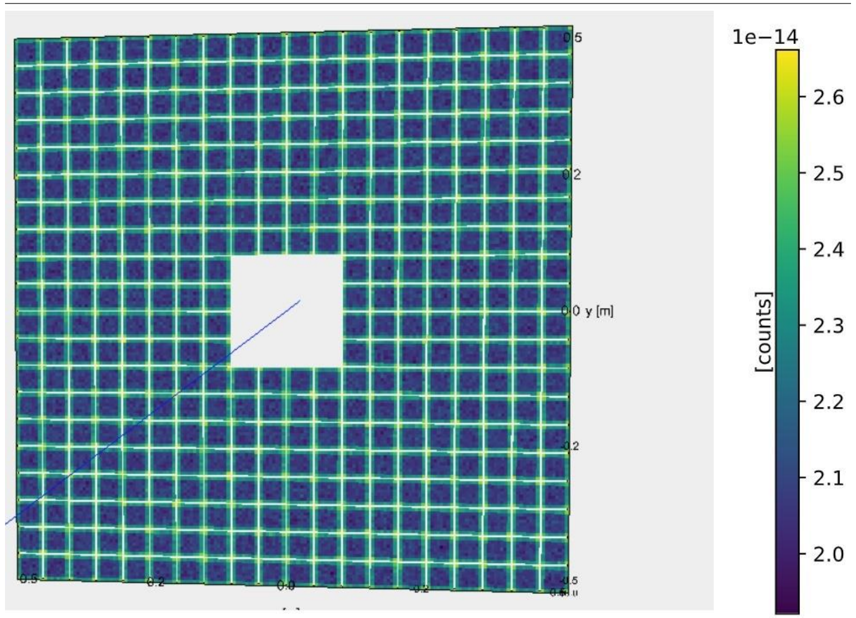
Codebase / simulation output

- Code Implemented as a Python package following the template for a McStas instrument project from Mads (https://github.com/mccode-dev/template_project)
- Repo: https://git.esss.dk/dmsc-instrumentmodels/skadi
  - Includes the SKADI McStas model (updated by Damian Martin Rodriguez)
  - Example Jupiter Notebook to build, run, and visualize
  - Documenting README files
- Building all 3 detector banks (optionally not all of them), and putting them in front of a minimal frontend (source+sample) for testing, or in front of the Skadi instrument model (replacing the simple detector model present)
- Simulation output: McStas NeXus file containing a list of neutron detection events for each pixel
- Nexus files can be loaded with the *mcstastox* python package to get a *scipp_object*

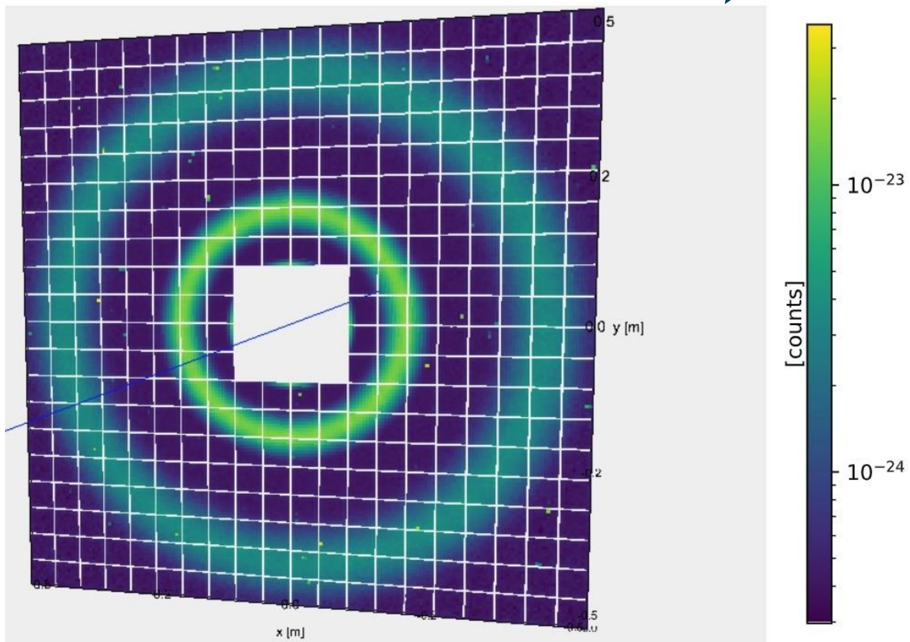
Output - demonstration

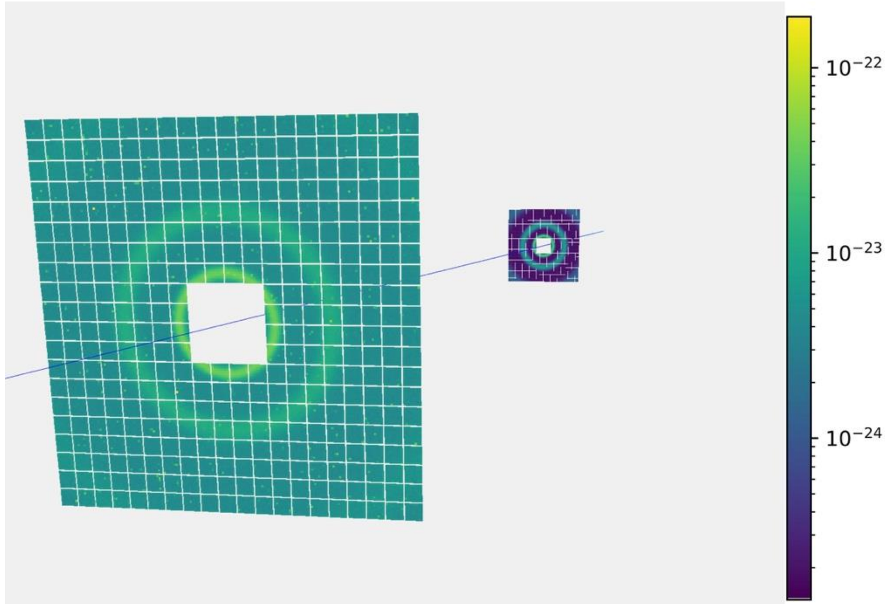
- Uniform parallel illumination single tile/front bank





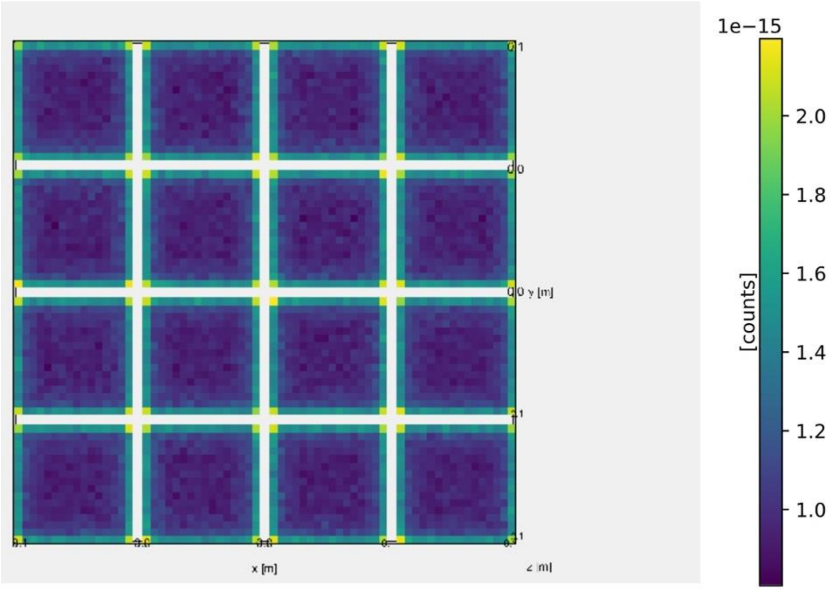
- Pencil beam of 6 Ang neutrons on a sample with sharp peaks (*SANS_benchmark2* model 10) 1 / 2 detector banks



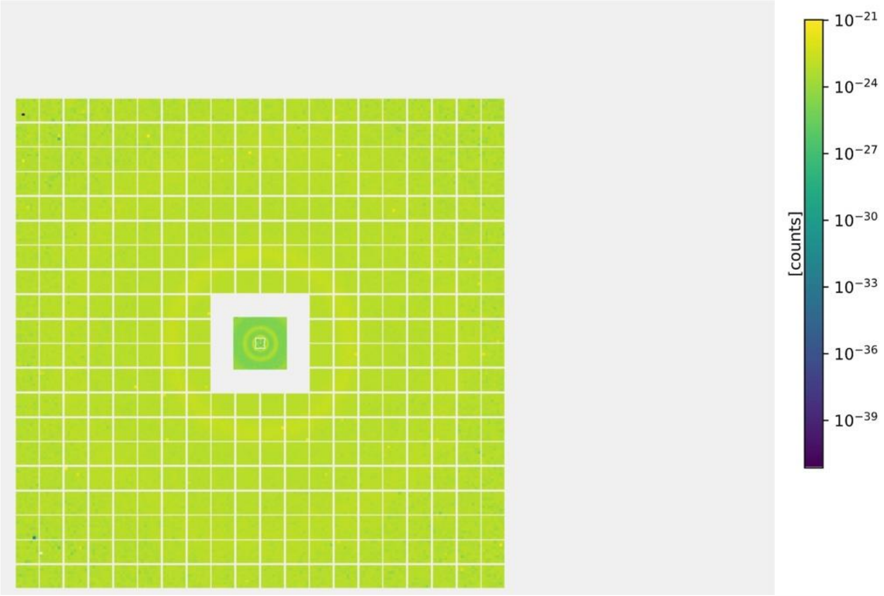


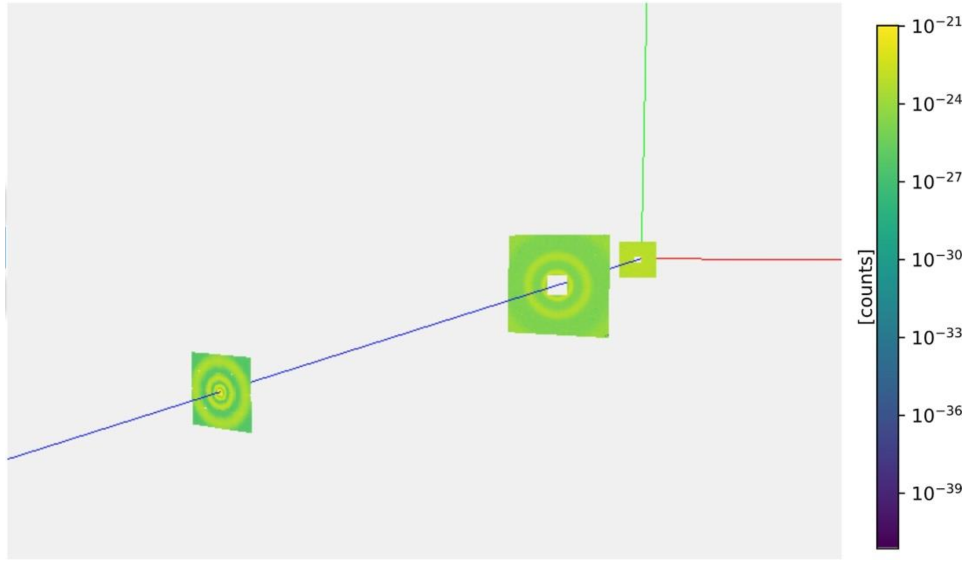
Progress - demonstration

- Uniform parallel illumination of the rear detector bank



- Pencil beam of 6 Ang neutrons on a sample with sharp peaks (*SANS_benchmark2* model 10) all 3 detector banks



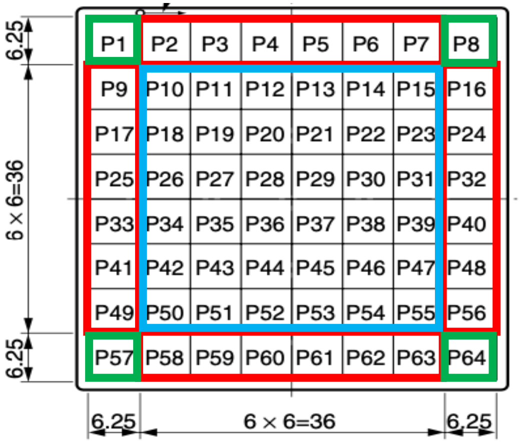


Outline

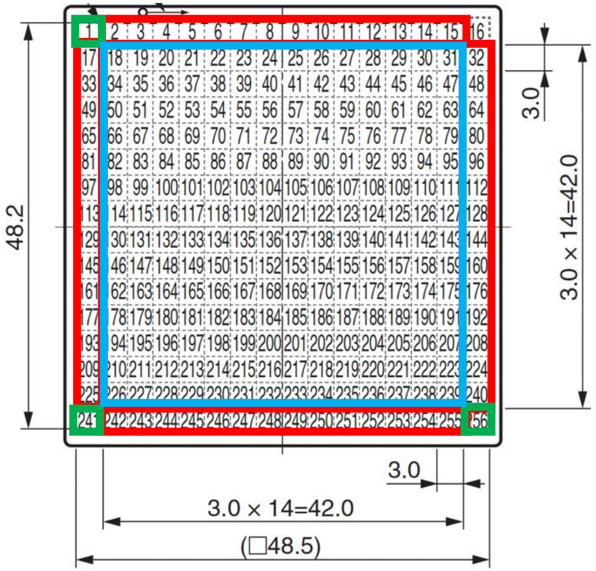
- SoNDe Geant4 simulation
- McStas model implementation
- **The challenge on the non-uniform pixel sizes**
- The challenge of the pixel ids
- Planned usages

Non-uniform pixel sizes

- A single detector consists of 3 different sized pixels, different for front/middle and rear bank.
  Corner pixels / **Edge pixels** / **Inner pixels**



8x8 VS 16x16 pixels

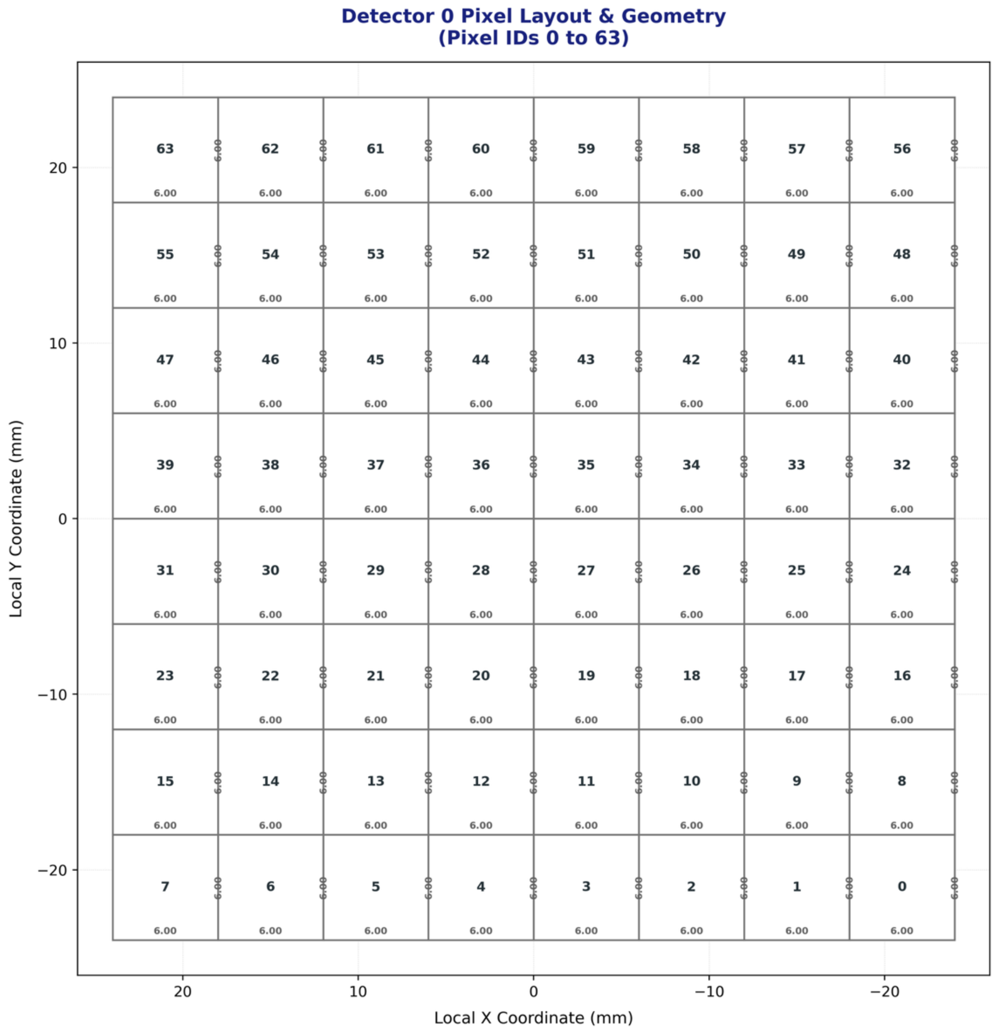


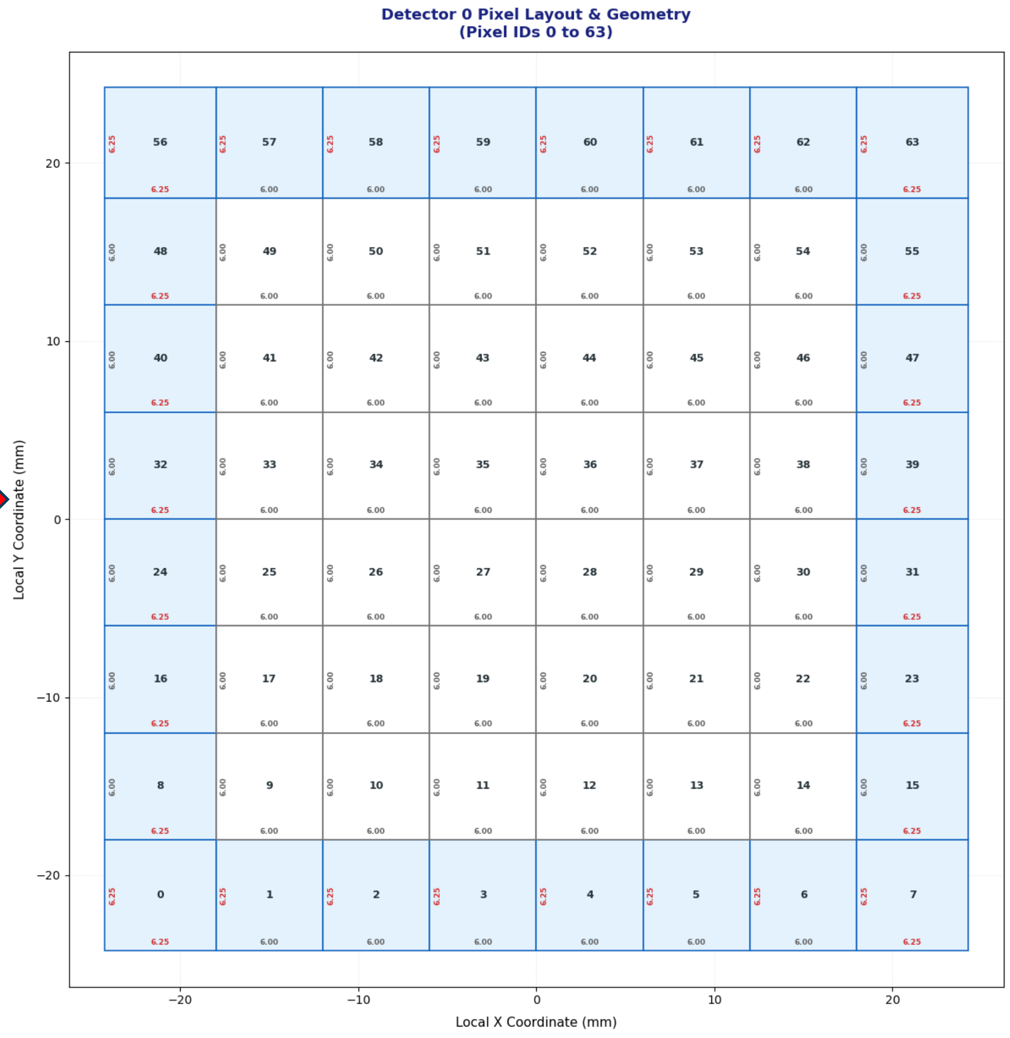
- Only uniform bin size is allowed for *monitor_nD* (that is used in the monitor comp)
- 6/3 mm pixels are used, but absorption events on the outer perimeter of the detector (0.25mm) are moved inside the pixel by 0.25mm, so they are added to the histogram
- The output NeXus file has **wrong pixel position for the pixels on the perimeter**!

- The ultimate solution: use the ECDC NeXus/JSON geometry for data reduction

Non-uniform pixel sizes

- Temporary solution: fix the pixel position of the *scipp_object (Coded with AI help)*



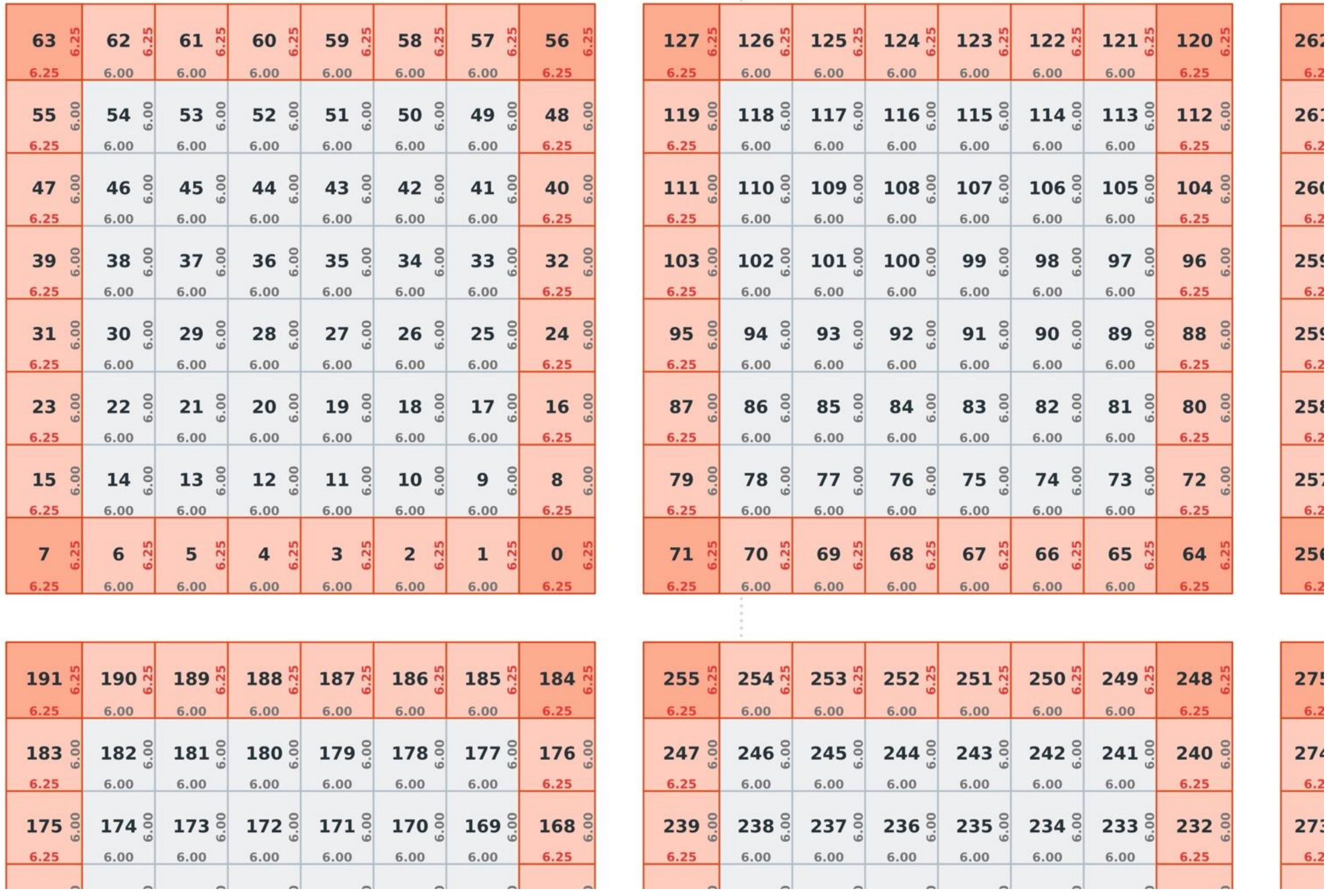


Non-uniform pixel sizes

- Seems to be working for the full geometry

- AI made tests to check
  - New sizes
  - No overlaps
  - Pixel centre distances
  - Distances between detectors
  - …

- TODO check the test :)…



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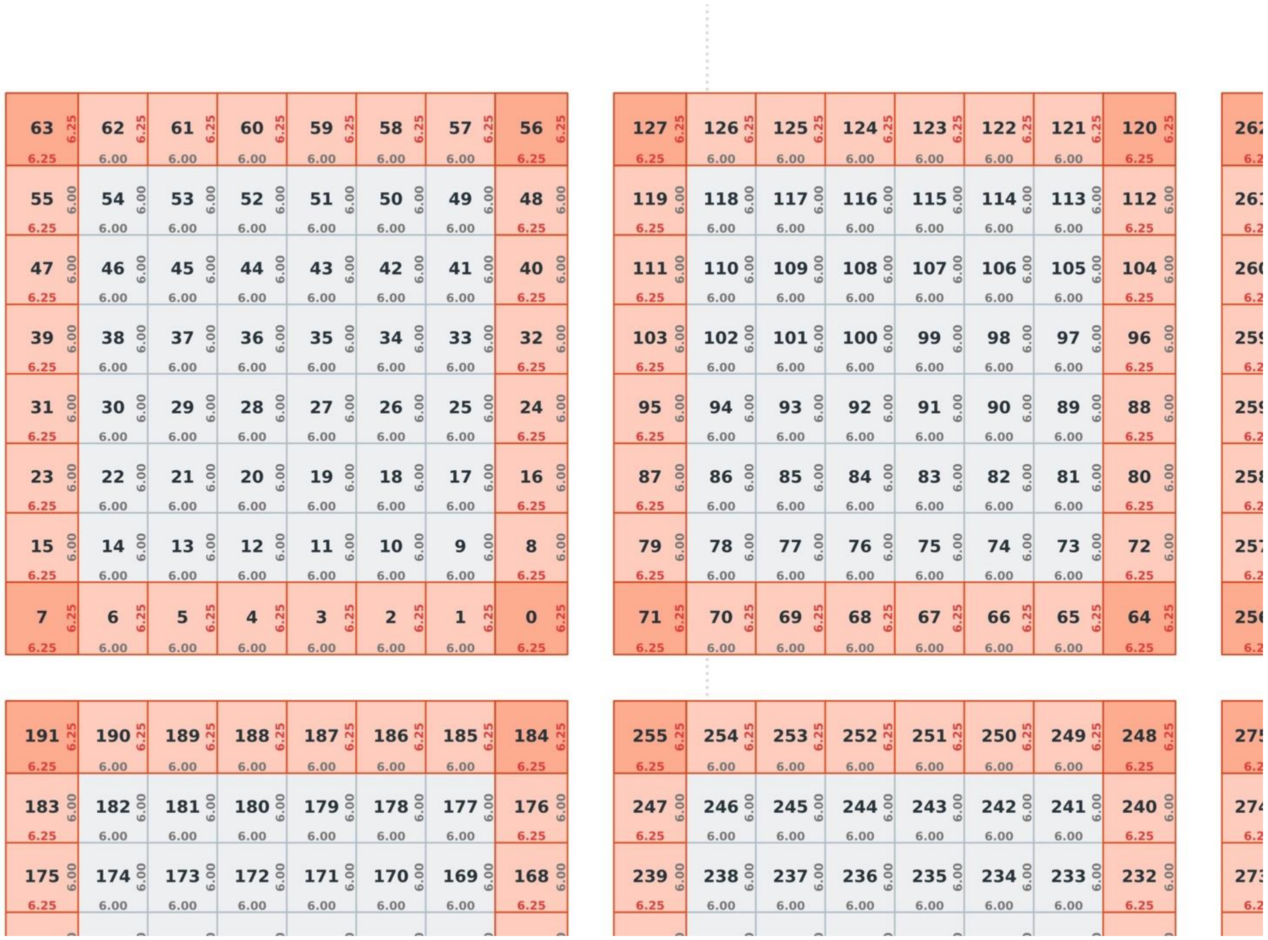
Pixel ids

- Pixel id order is not defined yet
  - Pixel order within a detector
  - Order within a tile (2x2 detectors)
  - Order among tiles (detector bank)
  - Order among banks

- In the McStas model the order of the monitors decide the order of the pixel ids
  - currently it's quite arbitrary
  - I might follow what is decided, or map pixel ids after the simulation



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Planned usage

- Generate simulated data for the data reduction workflows in Scipp readable format
- Simulate:
  - Different instrument (frontend) settings
  - Different samples
  - Different bank positions
- Maybe help the ECDC Nexus/JSON detector definition
- Note: it was planned to be used for studying scattering effects, but the model lacks structural components, absorber layers…
- Note: due to the large number of monitors (and buffers required for the monitors), the model can be heavy for personal computers/laptops! (DMSC Cluster needed)