Update from BIFROST, CSPEC

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DMSC

2023-04-26 DMSC STAP

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Overview

- Recapitulation
- Plans

Setting up BIFROST McStas simulations

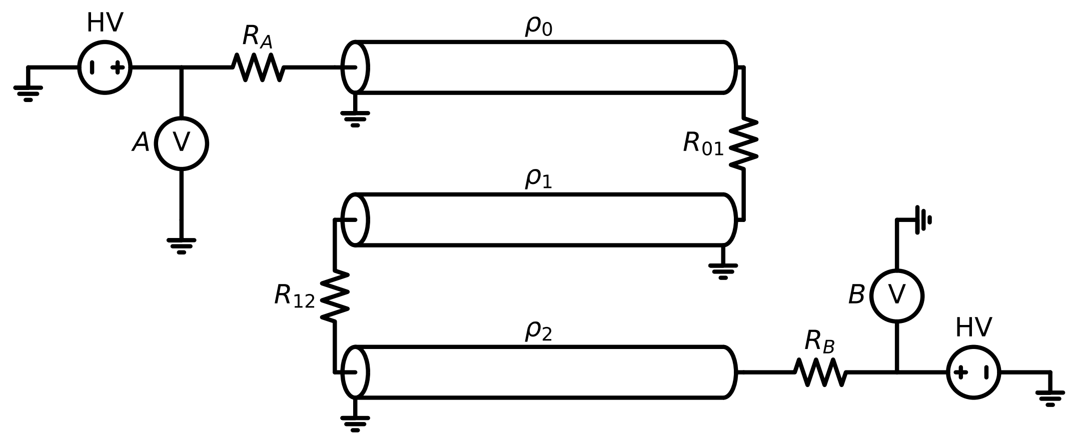
Motivation

- BIFROST is the first CAMEA Time-of-Flight spectrometer
- Need realistic data to test workflows
    - data transformation
    - instrument calibration
- Faithful simulations could produce a *digital twin*

- Secondary spectrometer has 45 analyzer-detector *pairs*, 9 each for 5 final energies
    - 3 variants for each energy: short, medium, long

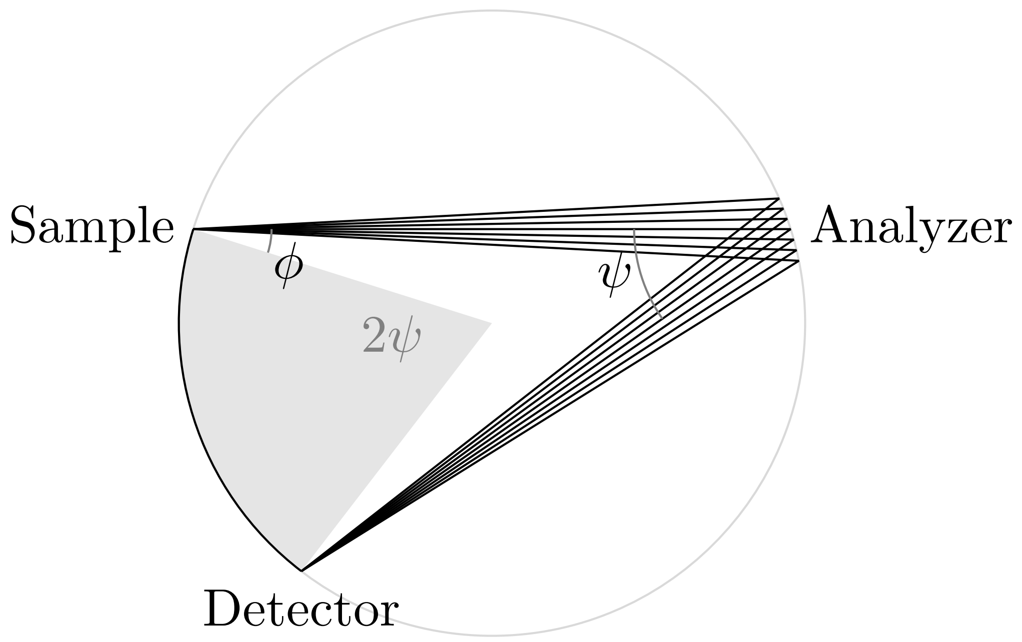
45 *triplet* tube ^{3}He detectors with anode wires in series

Three detectors connected in series to form a *triplet*.



45 *Rowland* geometry 7- or 9-blade focusing analyzers

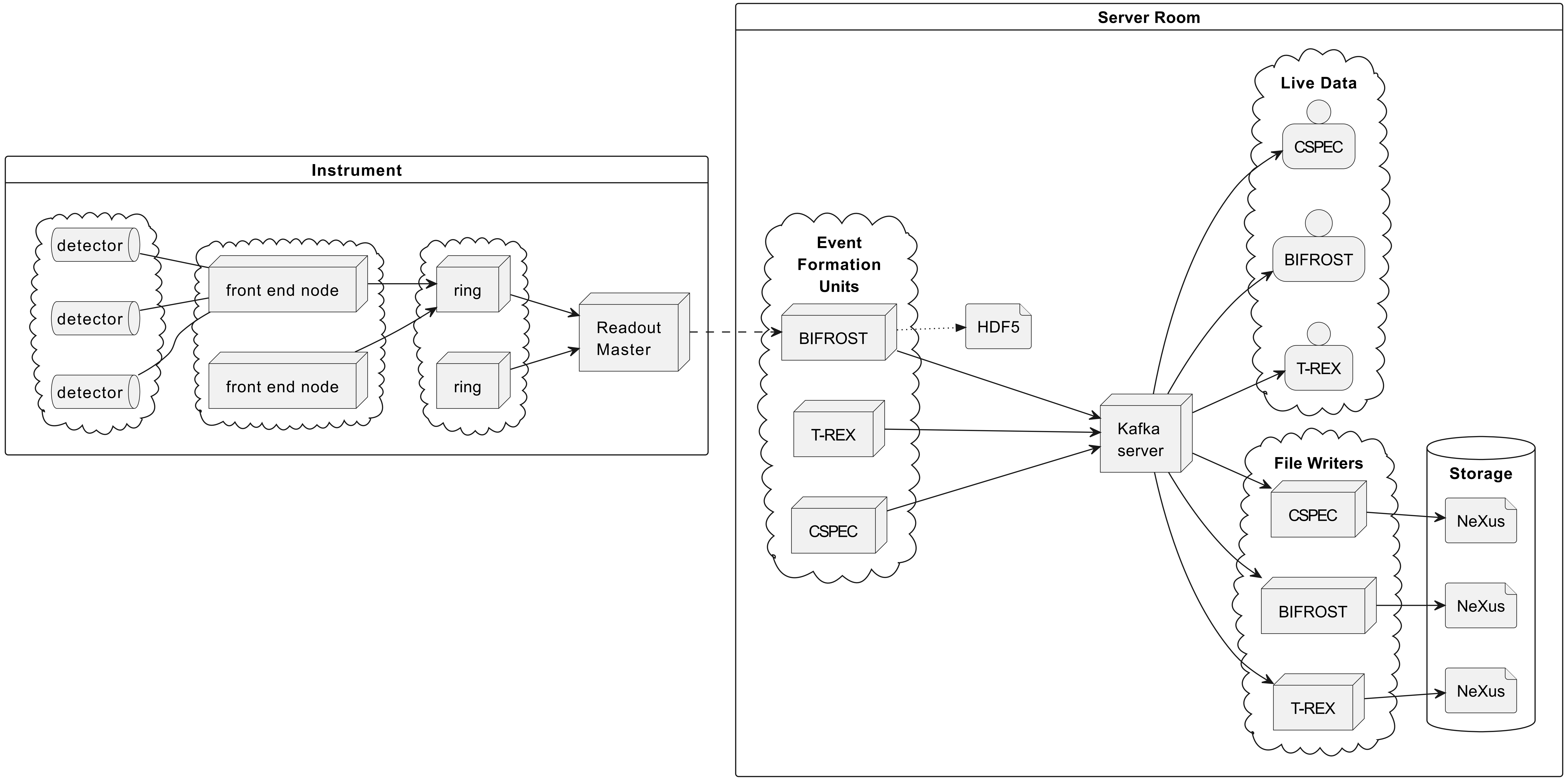
Pyrolytic graphite crystals are arrayed on the surface of a cylinder along with the sample center and triplet center.



Classic McStas components would require 135 `Monitor` and 369 `Monochromator` components.

Data collection via readout chain

Data from the instrument is of the form `(A, B, TUBEid, FENid, RINGid, EventTime, PulseTime)`.



The Event Formation Unit converts this to `(DetectorIndex, EventDeltaTime, PulseTime)` where the index identifies a logical pixel in one of the continuous position sensitive tubes.

Prior McStas Models of BIFROST

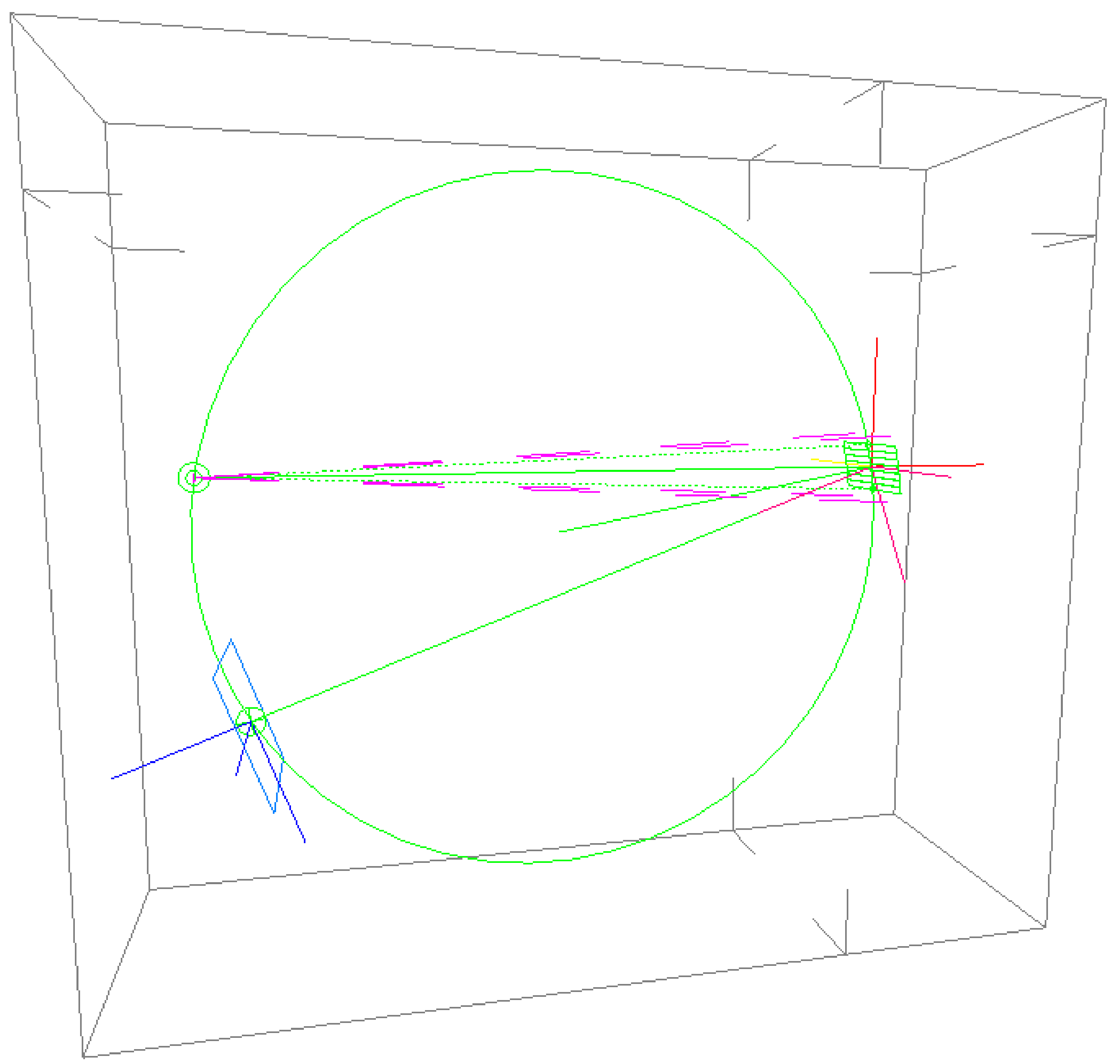
- A definitive primary spectrometer
  - 1675 line instrument file
  - includes choppers and guides from source to sample
- Various partial implementations for the secondary spectrometer in McStas v2
  1. 5942 lines, implementing 5 analyzer-detector pairs over 9 instrument files
  2. 6105 lines, implemented over 3 instrument files

The earlier secondary spectrometer simulations:

- Did not simulate the Readout Master data
- Used 2-D PSD or three 1-D PSD monitors in place of the triplet detectors
- Could not simulate the entire backend simultanously
- Are complicated to read through or modify due to their length

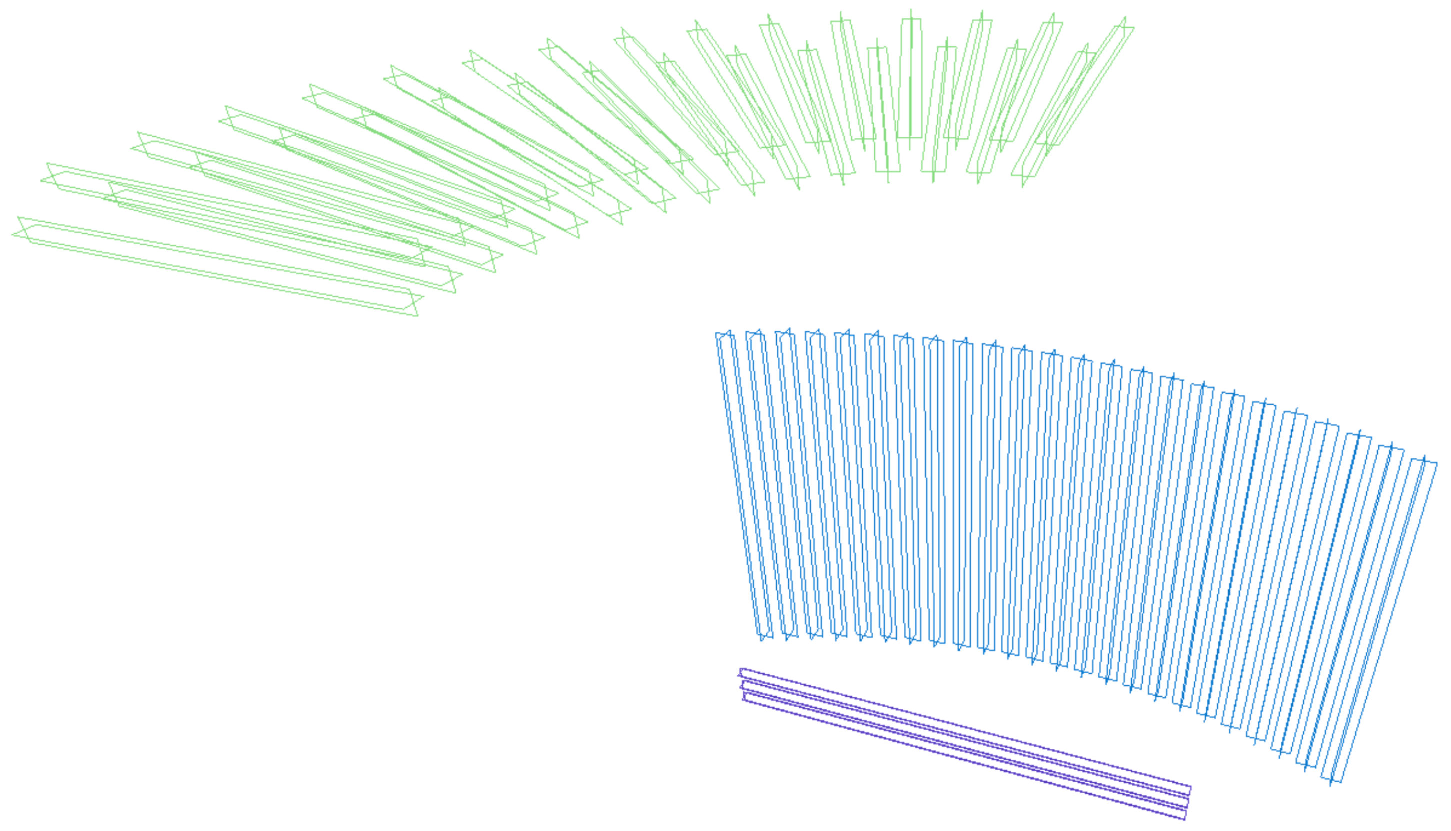
Rowland Geometry monochromator component

- Each analyzer is one component instead of 7 or 9 individual blades
- Calculates Rowland circle from own position and *source* and *focus* component names
- Places N equivalent crystals and optionally adjusts orientation for focusing



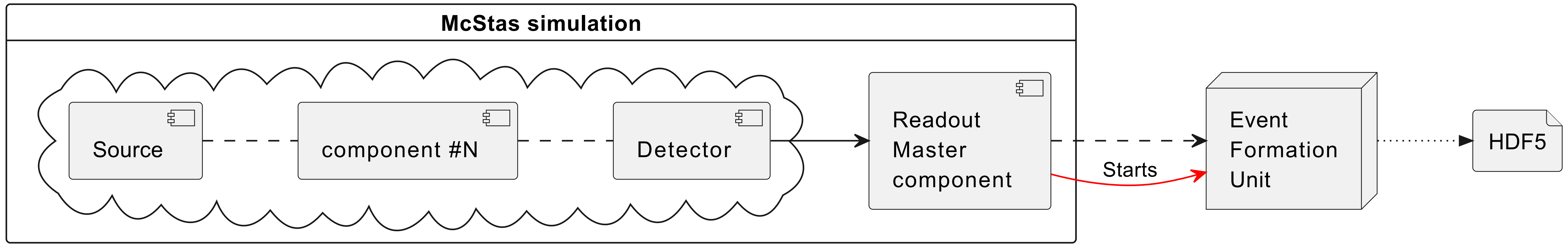
Detector_tubes monitor component

- One or more cyllindrical ^{3}He detector tube in series or parallel
- Simulates detector physics and readout electronics, producing `(A, B, EventTime)` per weighted neutron
- Parameters control
    - position, size and orientation of each tube
    - per-tube wire resistivities
    - inter-tube resistor values
    - contact resistances
    - reduced response end-tube regions

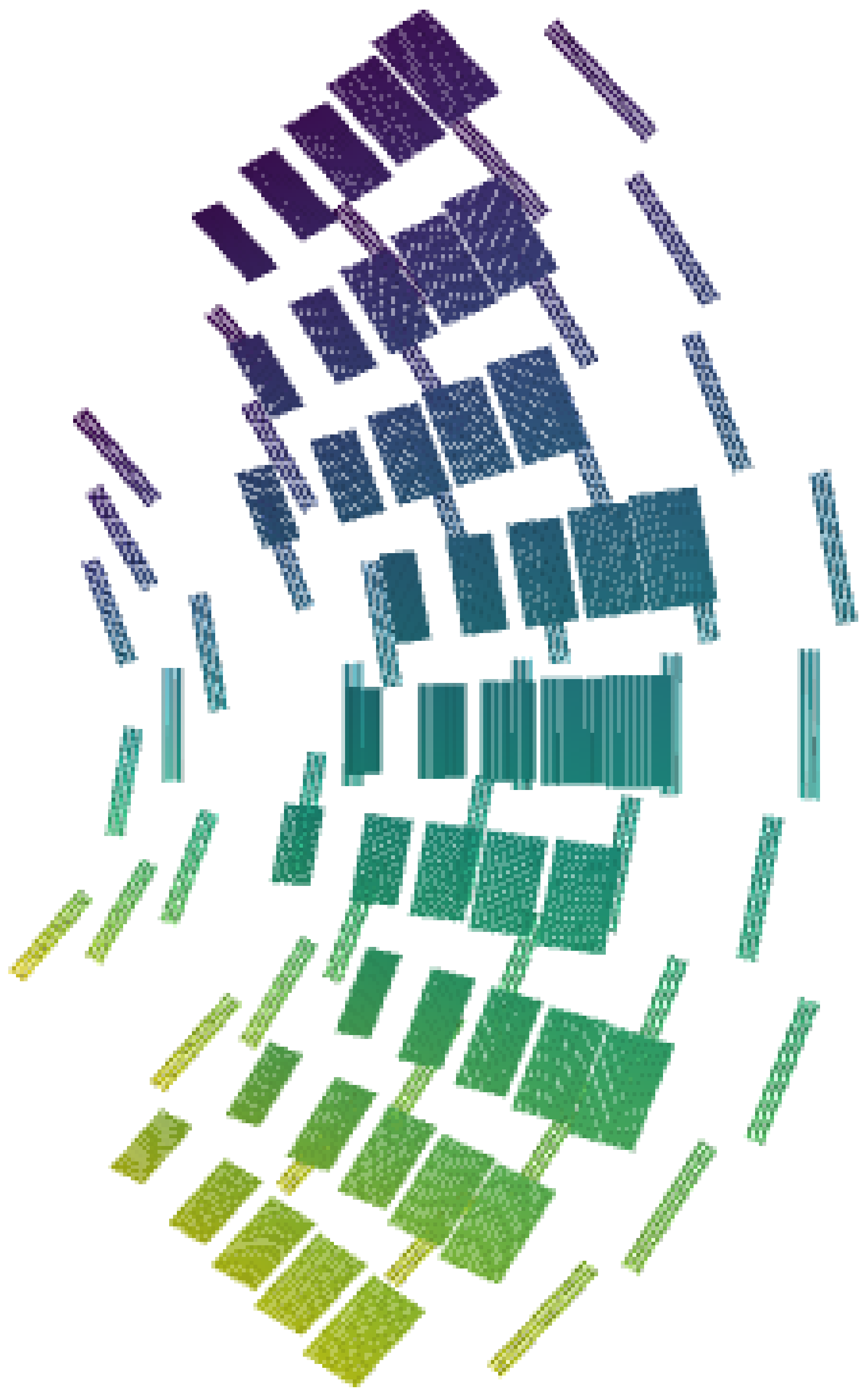


Readout Chain

- Readout Chain logic in instrument file
    - Extending components allows appending `(TUBEid, FENid, RINGid)` to detected weighted neutrons
- New Readout Master component
    - Collects weighted neutrons and uses Poisson distribution to produce events
    - Collates network packets in ESS format
    - Sends full packets to an Event Formation Unit
    - Optionally, starts and stops a local EFU to enable `mcrun` based instrument parameter scans



Python-McStas BIFROST spectrometer



- Positions and orientations from calibration
- Uses (modified) McStasScript to insert custom components into a McStas v3 instrument

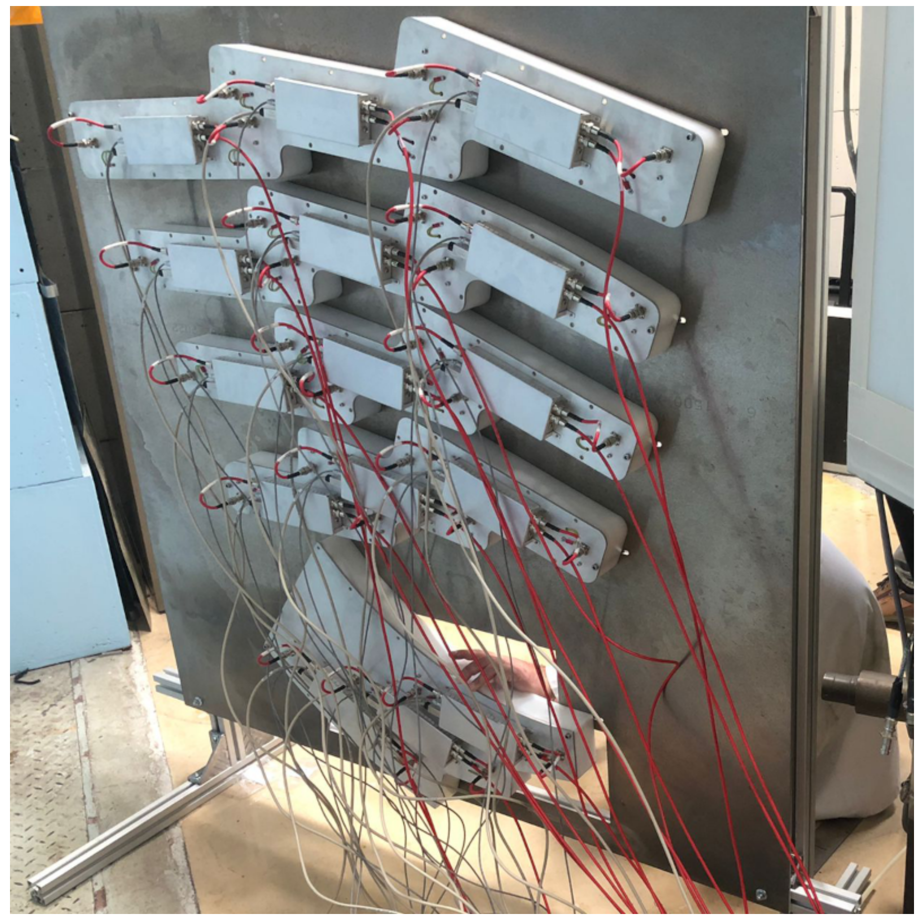
Progress

- Simulations with one analyzer-detector pair and a moveable slit
- Full instrument simulations, including a McStasScript primary spectrometer
- Simulations can run under MPI for parallelism and can use MCPL to increase data-packet rates

Availabile on GitHub

Component	**under https://github.com/g5t**
Rowland analyzer	mcstas-monochromator-rowland
Multiple ^{3}He detector	mcstas-detector-tubes
ESS readout master	mcstas-readout-master
BIFROST & CSPEC models	instrument-components

BIFROST detector tests @ LLB



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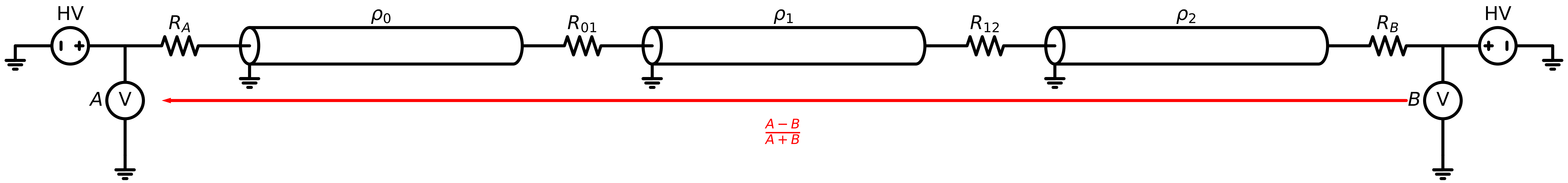
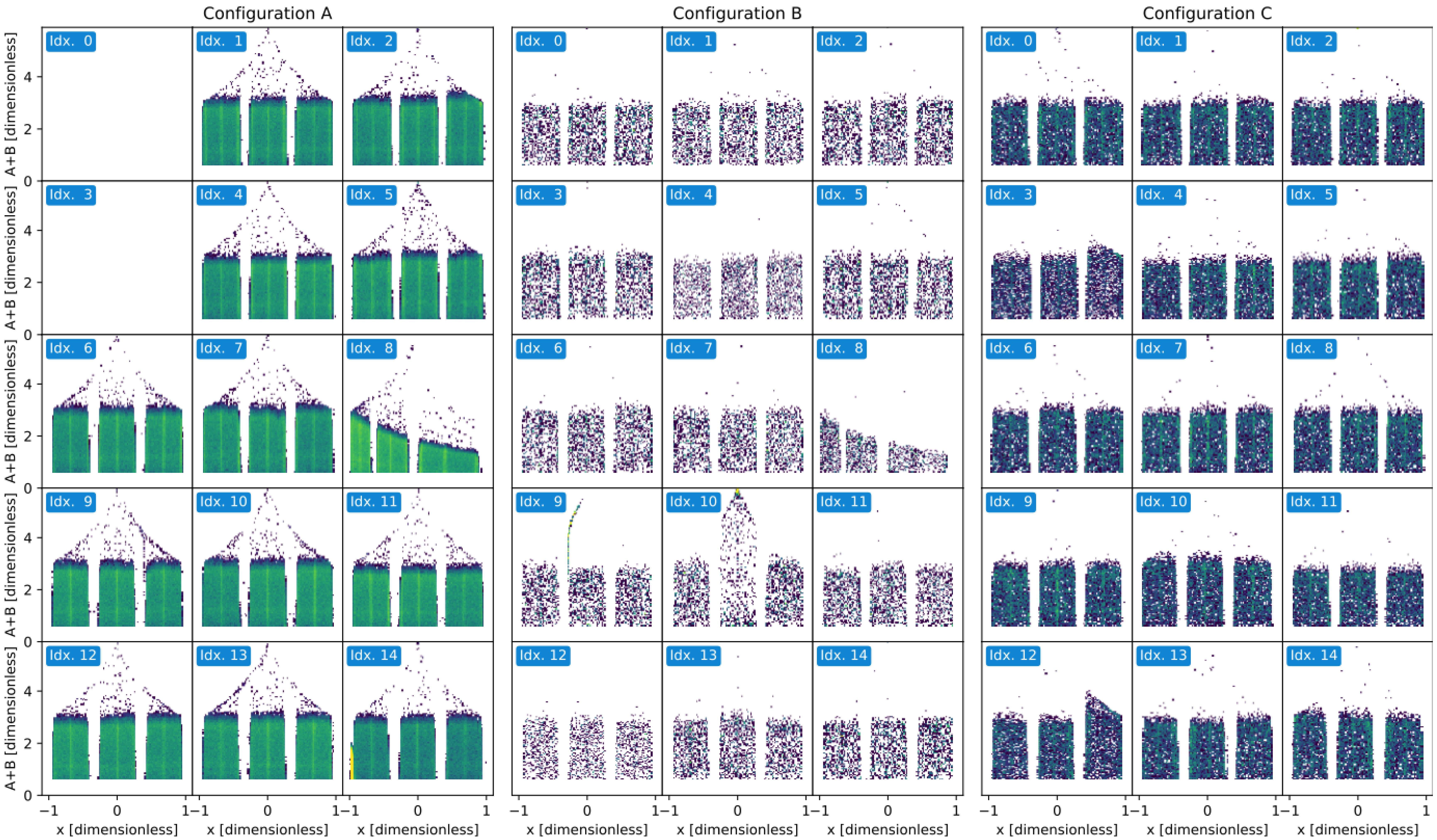
- Costruzioni Apparecchiature Elettroniche Nucleari (CAEN) R5560 + ILL firmware 'raw' data file format:
    - `{TimeHigh:32, TimeLow:32, Reserved:16, Channel:8, ID_Flags:8, A:16, B:16, Align:32}`

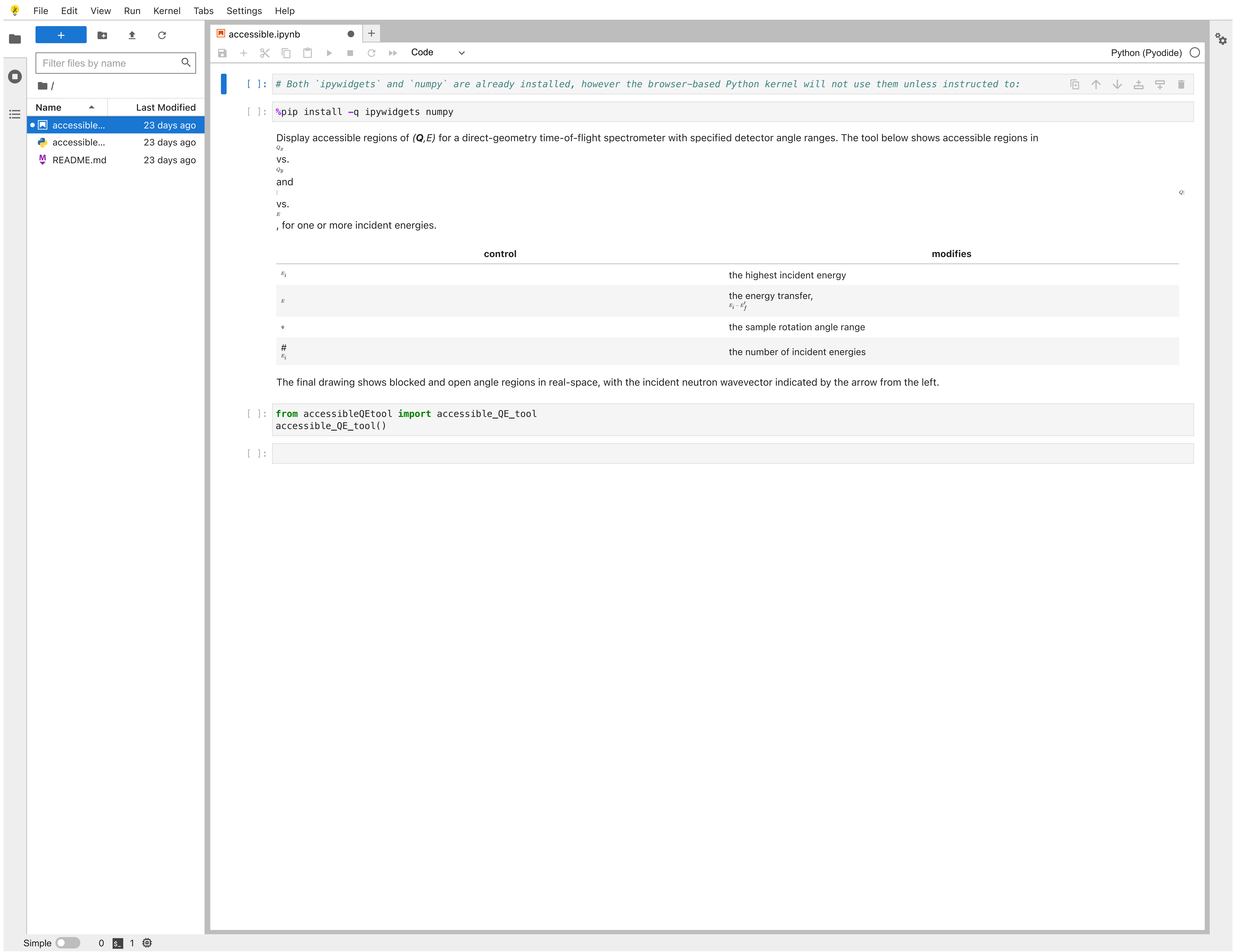
11101100000110000000000000000000000000000000000010010001000010011111111001000111010000000000000000000000000000000000

- `A+B` ∝ peak area
- Comparing `A` and `B` gives event postion along the *wire path*



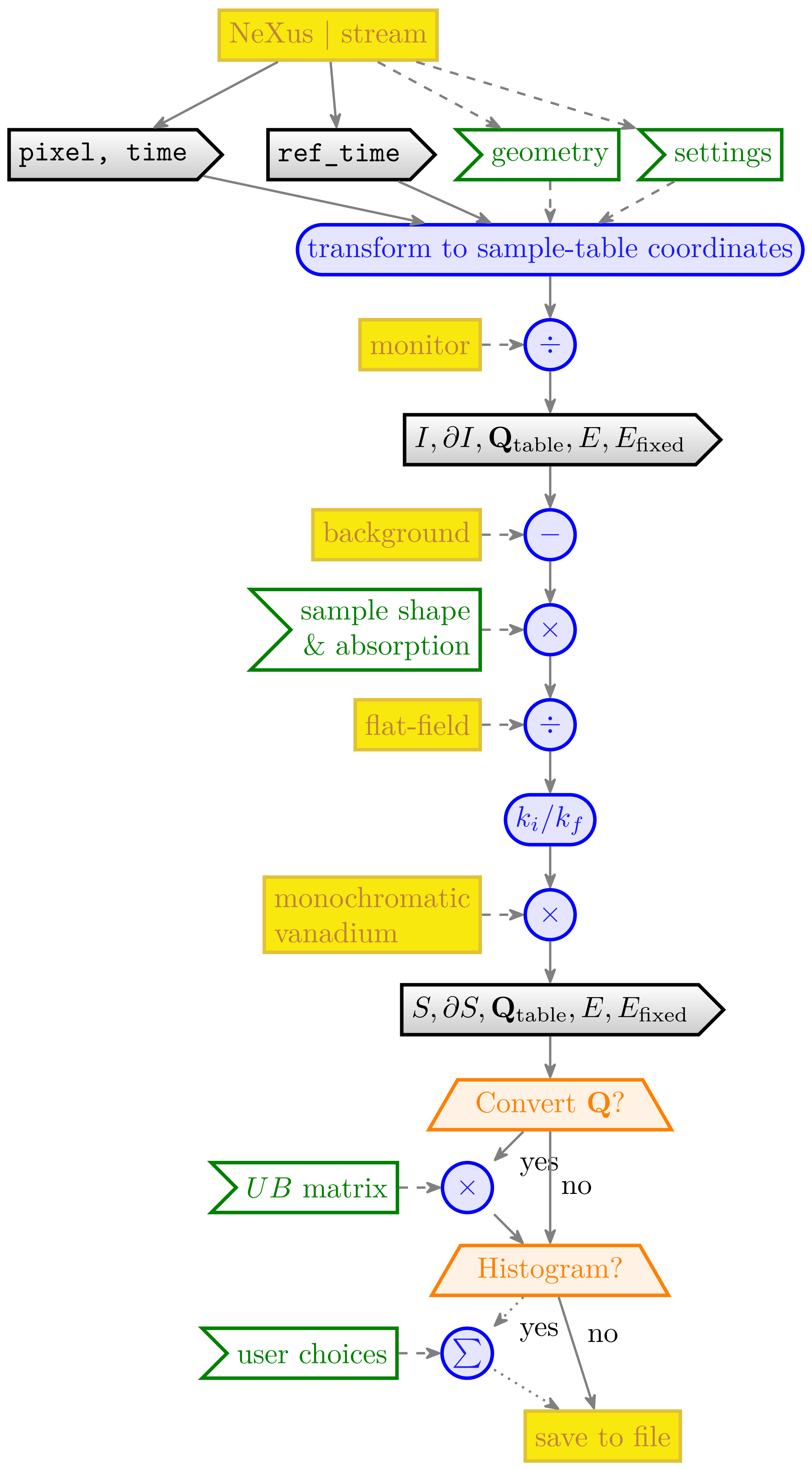


- The Event Formation Unit will only retain a subset of `x` from `A` and `B`
  - Is it sufficient to check diagnostic information only intermittently?
- Charge-division position from $\frac{A}{A+B}$ or $\frac{A-B}{A+B}$
  - How *should* we calculate position?



File Edit View Run Kernel Tabs Settings Help
Filter files by name
/
Name
Last Modified
accessible...
23 days ago
accessible...
23 days ago
README.md
23 days ago
accessible.ipynb
Code
Python (Pyodide)
[ ]: # Both `ipywidgets` and `numpy` are already installed, however the browser-based Python kernel will not use them unless instructed to:
[ ]: %pip install -q ipywidgets numpy
Display accessible regions of (Q,E) for a direct-geometry time-of-flight spectrometer with specified detector angle ranges. The tool below shows accessible regions in
vs.
and
vs.
, for one or more incident energies.
control
modifies
the highest incident energy
the energy transfer,
the sample rotation angle range
#
the number of incident energies
The final drawing shows blocked and open angle regions in real-space, with the incident neutron wavevector indicated by the arrow from the left.
[ ]: from accessibleQEtool import accessible_QE_tool
accessible_QE_tool()
[ ]:
Simple
0
1

Data reduction plans



Output of histogram or events to useful file formats:

type	format	defined by
histogram	NXspe	NeXus
	SQW	Horace
	HDF5	MJOLNIR
	small ASCII text	
event	HDF5	scipp
	MDWorkspace	Mantid
	whole-experiment format	

Should we support any additional formats?

Data analysis plans

Aim to support users to make use of software including DAVE, PACE, Mantid, *LAMP*

area	**software**
powder	MSlice, OCLIMAX
single-crystal	Horace, SHIVER, MJOLNIR
QENS	*interface to QENS Model Library*, *STRfit*

Is this list appropriate?

First science ideas

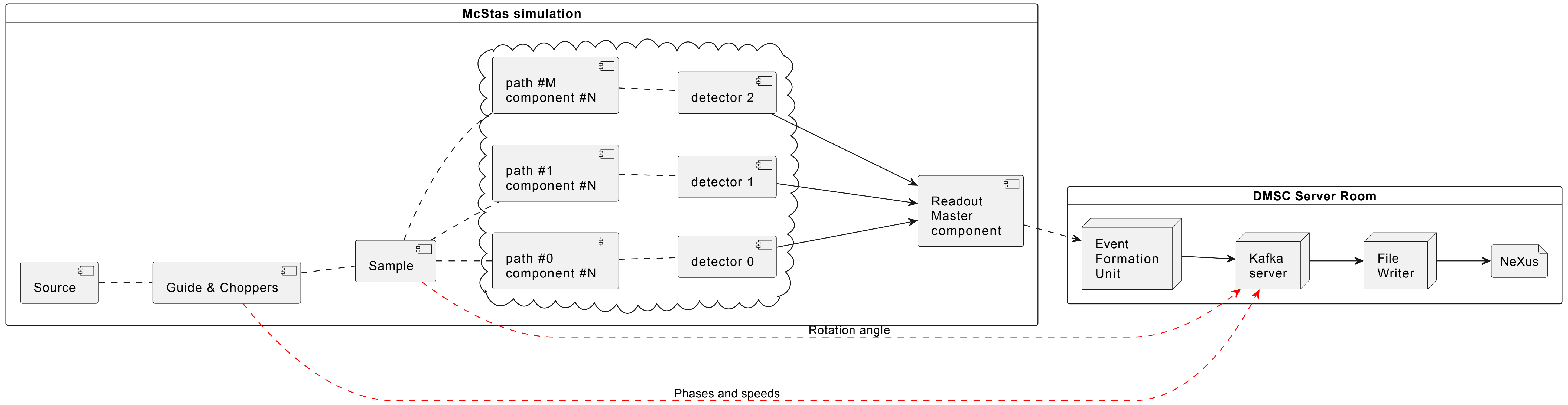
First Science experiments should produce

- data which is *simple* to transform
- transformed data should be *simple* to analyse
- → no known-complications & methods are defined *before* the experiment

General ideas, to be refined:

- Low-dimensional systems
- Existing measurements with insufficient resolution to answer key questions?
- Machine learning problems; similar to K T Butler et al J. Phys.: Condens. Matter 33, 194006 (2021) or A Samarakoon et al Commun. Mater. 3, 84 (2022) but trained in anticipation of experiment results?

Short-term



- Produce NeXus file(s) from the full simulation through the full readout-chain
- Simulate a BIFROST experiment
- Develop and test the data transformation workflow

Long-term

- Automatic generation (or retreival) of MCPL files once data-acquisition parameters are known, in order to
  - feed-into an acurate digital twin of the experiment
  - enable fast resolution calculations for model comparison
- Regular application of machine learning techniques to:
  - experiment control
  - data analysis

Questions?