



# Detector rate estimate for the BIFROST instrument

Milán Klausz

[Milan.Klausz@esss.se](mailto:Milan.Klausz@esss.se)

HAS Centre for Energy Research  
European Spallation Source ESS ERIC  
BUTE Institute of Nuclear Techniques

Detectors and Data Acquisition for Instruments Meeting,  
Paris, 12 February 2018

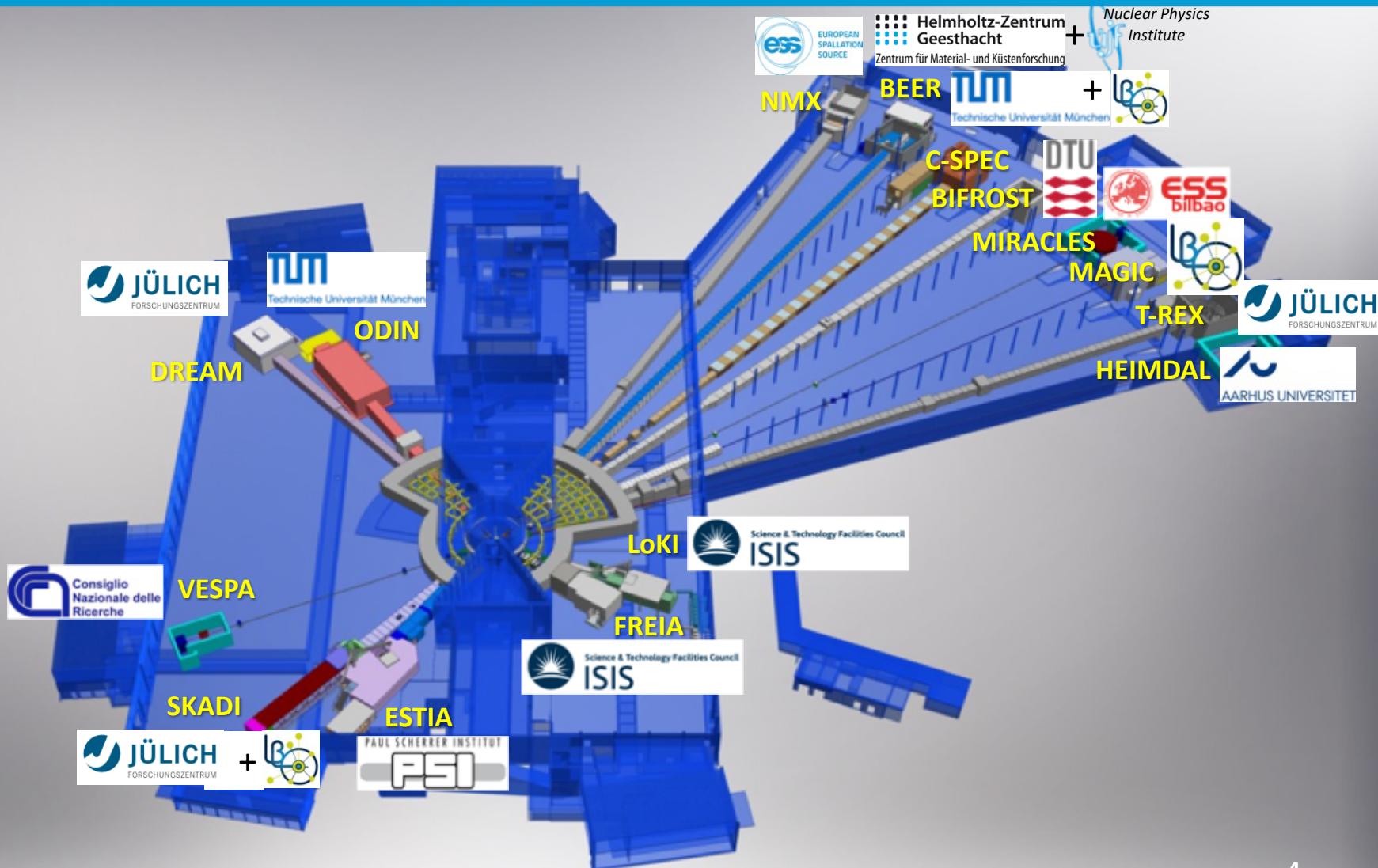
# Outline

- BIFROST Instrument
- Simulation Tools
- Simulation Model
- Results
- Outlook

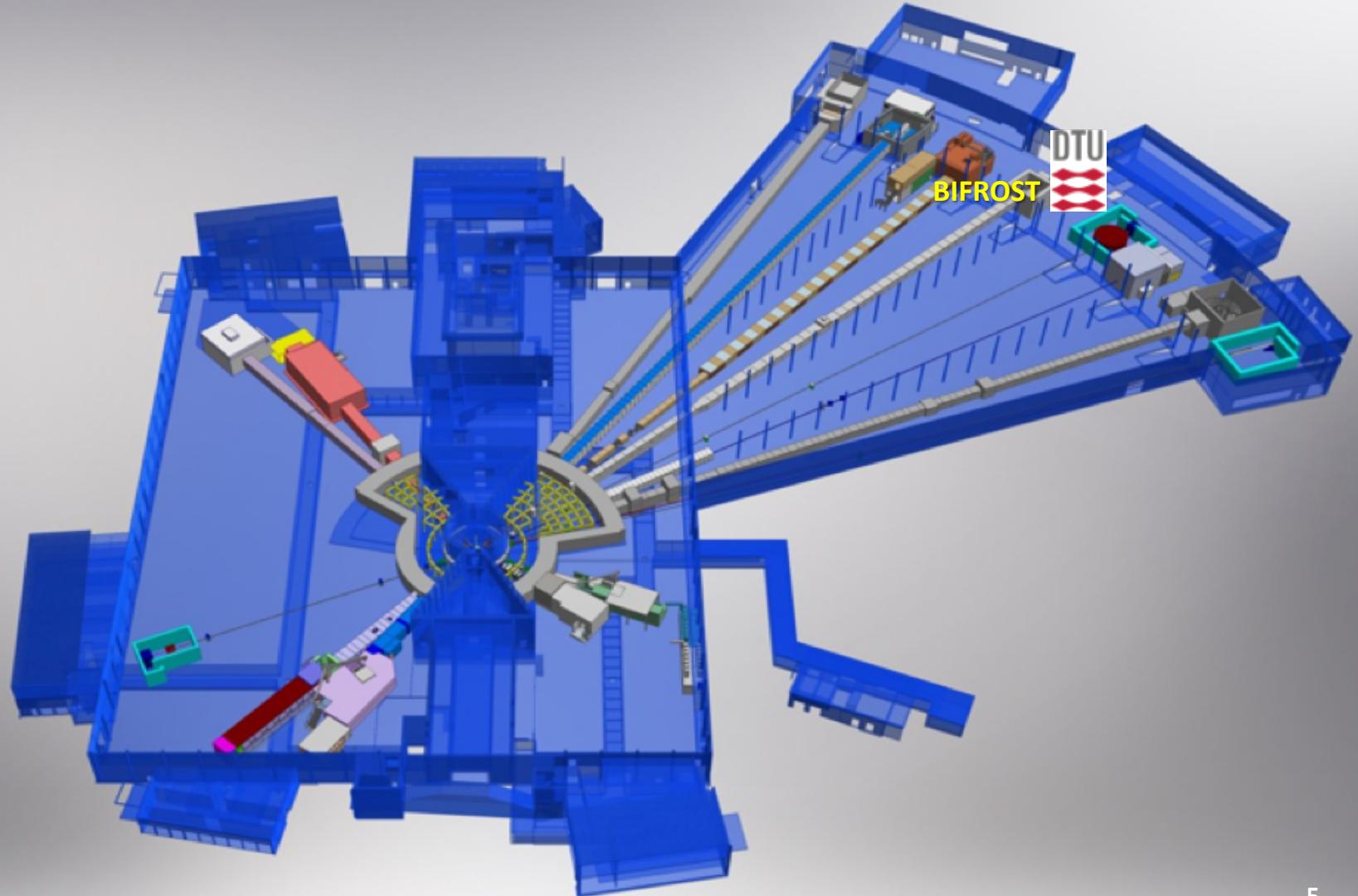
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# ESS - Instruments

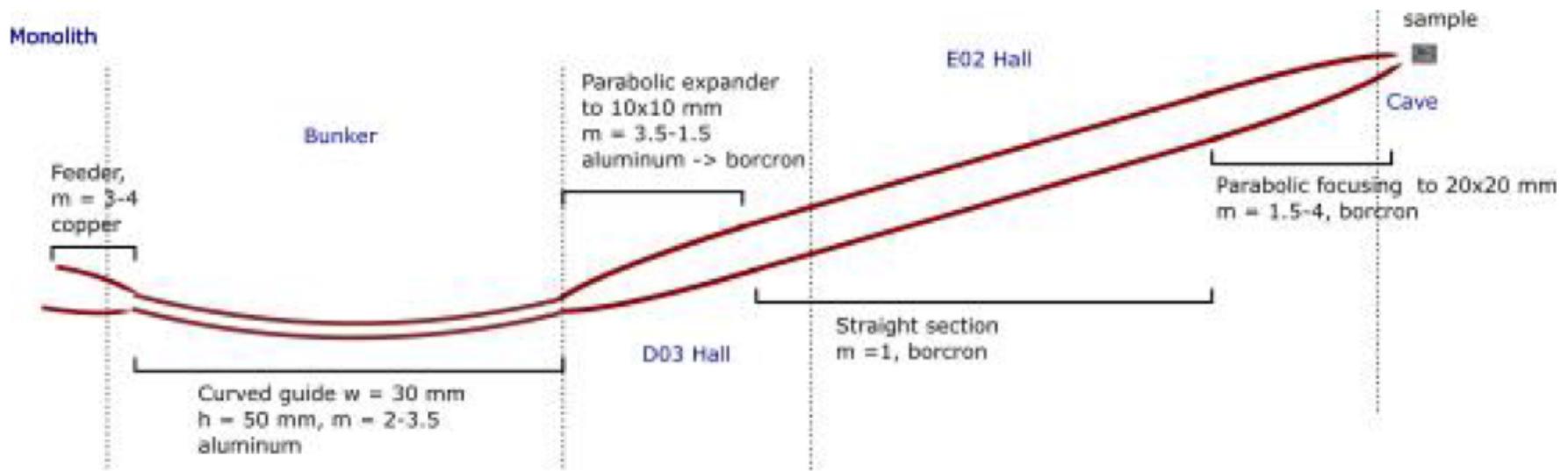


# Location of BIFROST



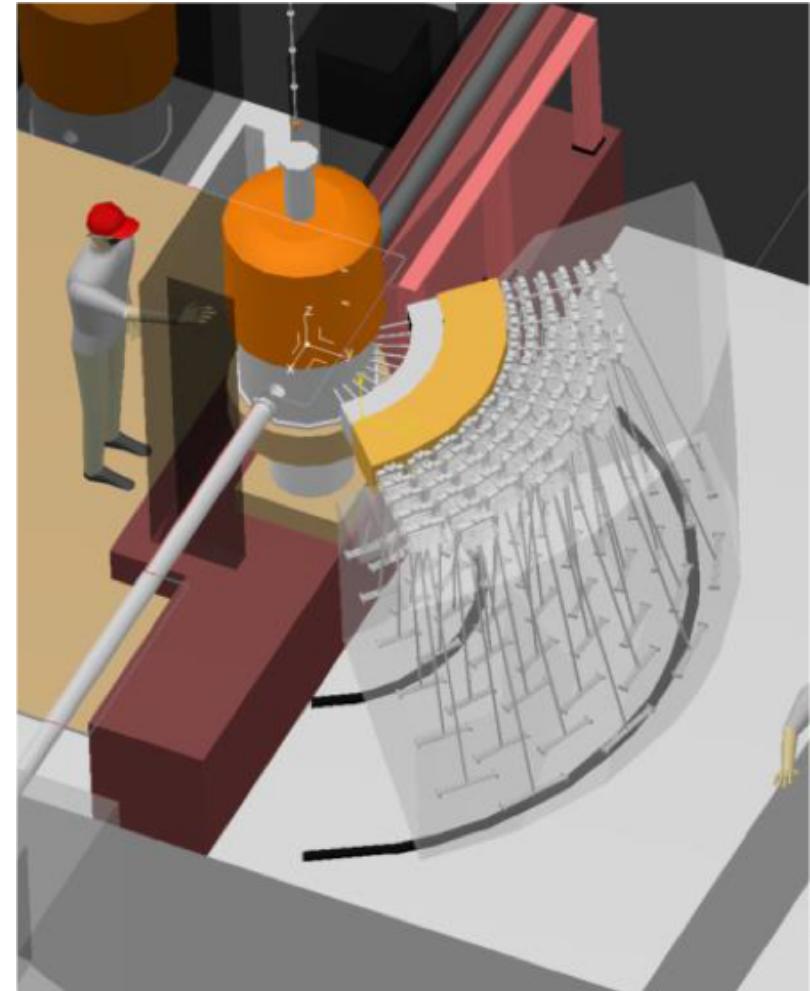
# Beam transport and conditioning system

- Curved guide section
- Copper blocks
- 4 choppers (PSC, FOC, FOC, BC)
- **Option to use full ESS pulse**



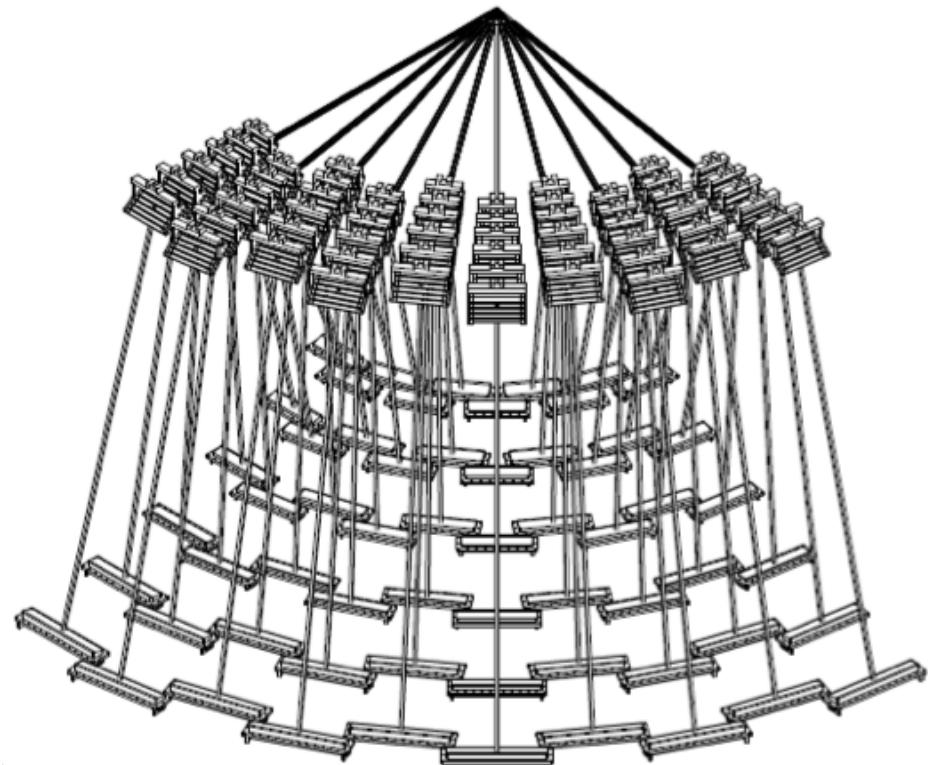
# Scattering Characterization System

- Filtering system
  - Beryllium filter
  - Radial collimator
- Secondary spectrometer tank
  - Vacuum vessel
  - Analyzers
  - Detectors and electronics
  - Crosstalk shielding
  - Tank positioning system



# Scattering Characterization System

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# Simulation Tools - Options



Guide

Sample +  
analyzers

Detectors

# Simulation Tools - Options

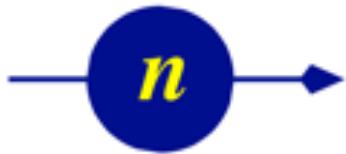


Guide

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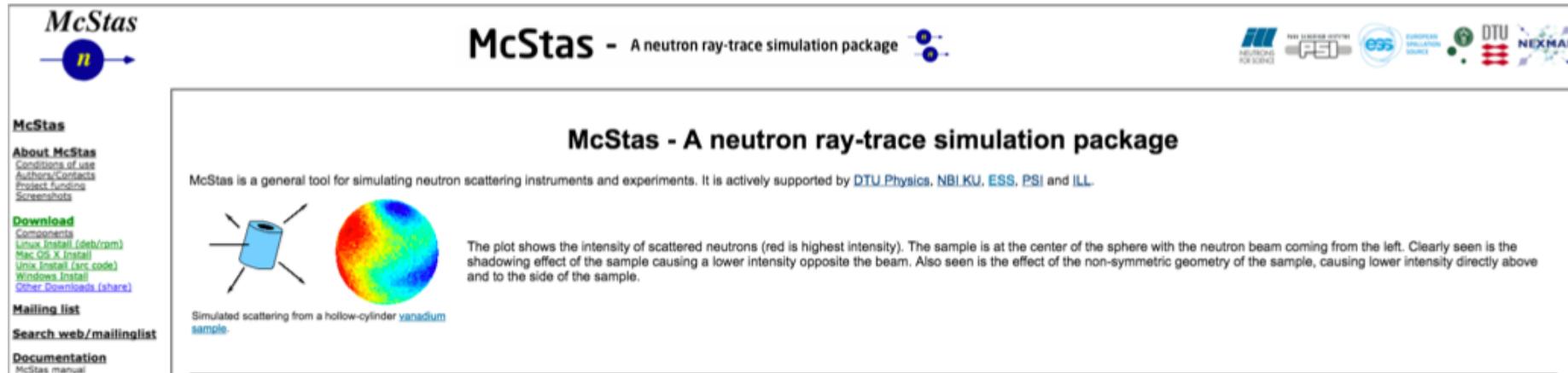
*McStas*



# Simulation Tools: McStas



- Simulation of neutron scattering instruments and experiments
- Monte Carlo ray-trace algorithm
- Cross-platform, open source
- Version 2.4.1 (Jun. 26, 2017)
- Collaboration:
  - DTU Physics
  - University of Copenhagen
  - Paul Scherrer Institute
  - Institut Laue-Langevin



The screenshot shows the official website for McStas. At the top left is the McStas logo, which consists of a blue circle with a yellow "n" and a blue arrow pointing right. The main title "McStas" is in large bold letters, followed by "- A neutron ray-trace simulation package". To the right of the title are four small logos: NBI KU, ESS, PSI, and ILL. On the far right, there are logos for DTU and NEXMAP. The left sidebar contains links for "About McStas" (Conditions of use, Authors/Contacts, Project Funding, Screenshots), "Download" (Components, Linux Install (deb/rpm), Mac OS X Install, Unix Install (src code), Windows Install, Other Downloads (share)), "Mailing list", "Search web / mailinglist", and "Documentation" (McStas manual). The main content area features a heading "McStas - A neutron ray-trace simulation package" and a paragraph explaining its purpose: "McStas is a general tool for simulating neutron scattering instruments and experiments. It is actively supported by [DTU Physics](#), [NBI KU](#), [ESS](#), [PSI](#) and [ILL](#)". Below this is a diagram showing a blue cylinder representing a sample and a circular heatmap representing scattered neutron intensity. A caption below the diagram reads: "Simulated scattering from a hollow-cylinder vanadium sample." A detailed description of the plot follows: "The plot shows the intensity of scattered neutrons (red is highest intensity). The sample is at the center of the sphere with the neutron beam coming from the left. Clearly seen is the shadowing effect of the sample causing a lower intensity opposite the beam. Also seen is the effect of the non-symmetric geometry of the sample, causing lower intensity directly above and to the side of the sample."

Source: <http://mcstas.org/>

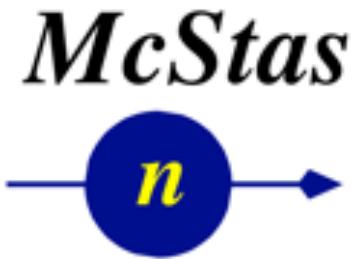
# Simulation Tools - Options



Guide

Sample +  
analyzers

Detectors



**Geant 4**

# Simulation Tools: Geant4 + DG Framework



- General purpose
- Developed in CERN
- Application in various fields
- Detector Group Framework
  - Code repository + build system
  - Tools, issue tracker, wiki
  - Geant4, C++, Python, Mercurial

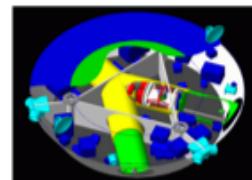
## Geant4

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The two main reference papers for Geant4 are published in *Nuclear Instruments and Methods in Physics Research A* 506 (2003) 250-303, and *IEEE Transactions on Nuclear Science* 53 No. 1 (2006) 270-278.

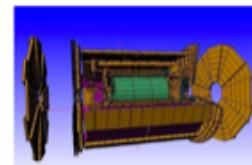
### Applications



### User Support



### Publications



### Collaboration



[A sampling of applications, technology transfer and other uses of Geant4](#)

[Getting started, guides and information for users and developers](#)

[Validation of Geant4, results from experiments and publications](#)

[Who we are: collaborating institutions, members, organization and legal information](#)

Source: <http://geant4.cern.ch/>

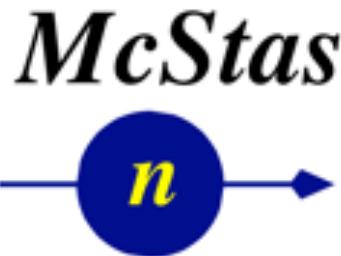
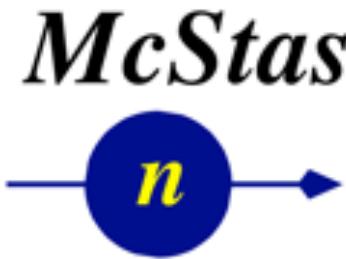
# Simulation Tools - Options



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Sample +  
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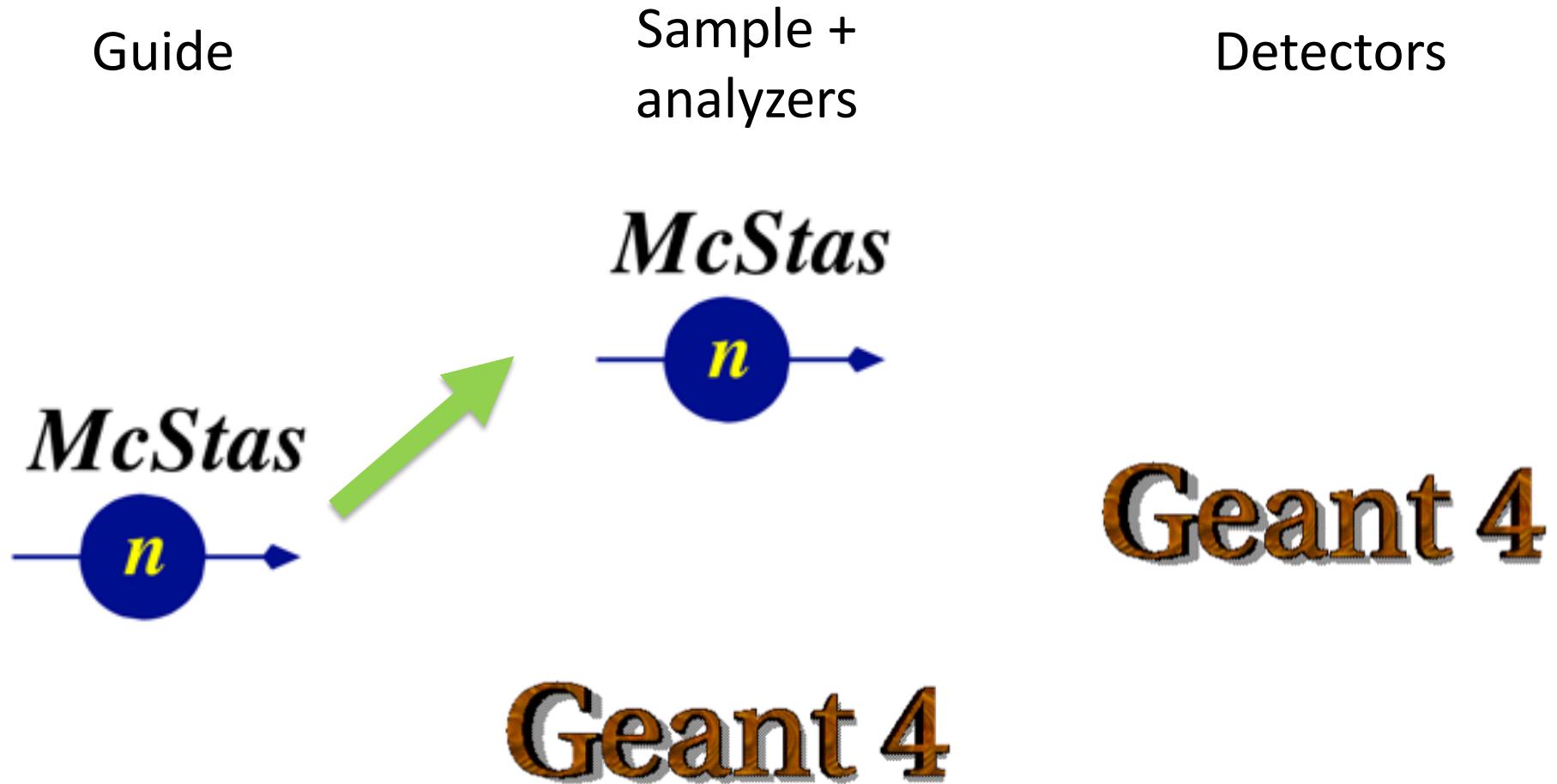
Detectors



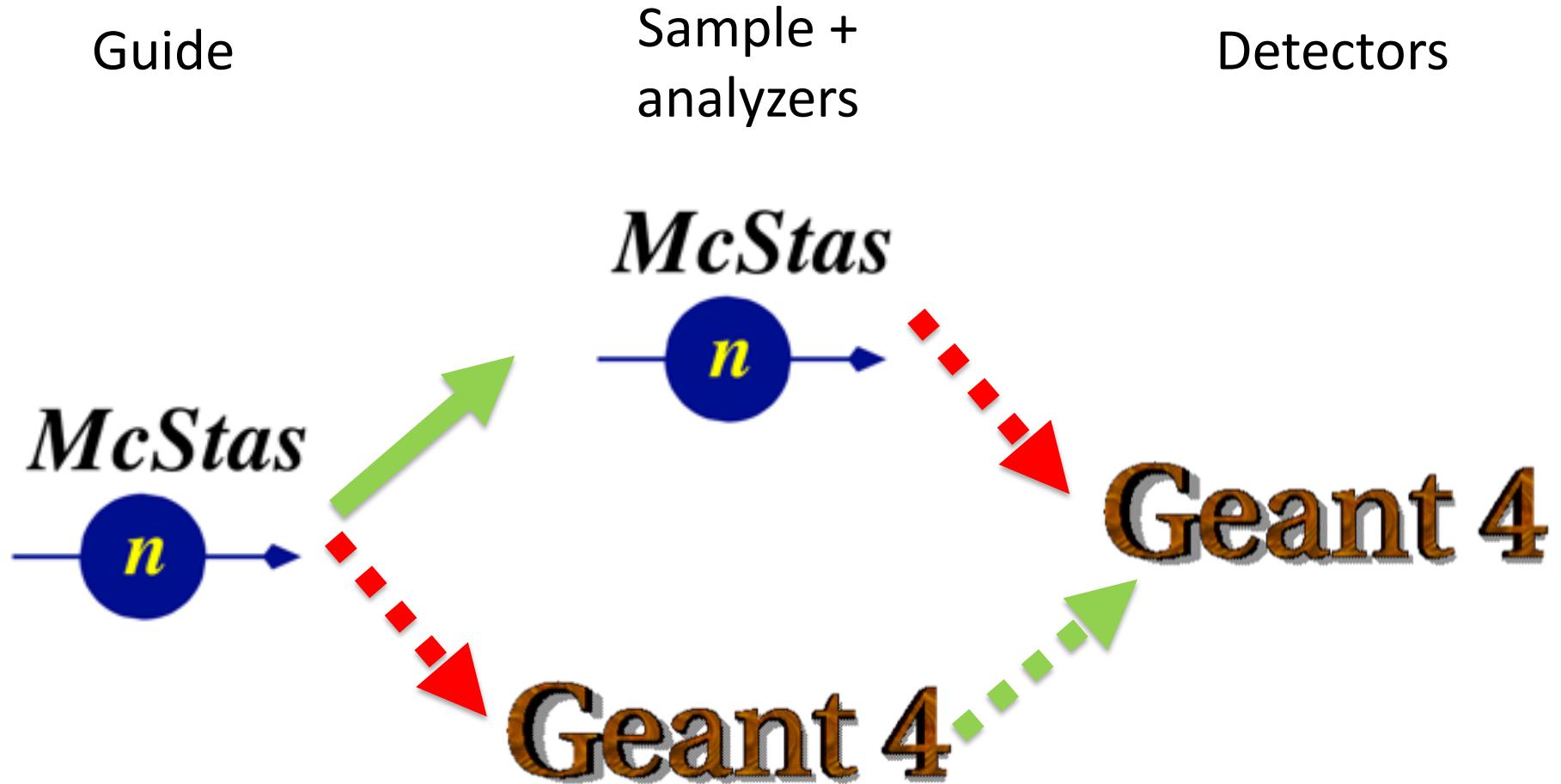
**Geant 4**

**Geant 4**

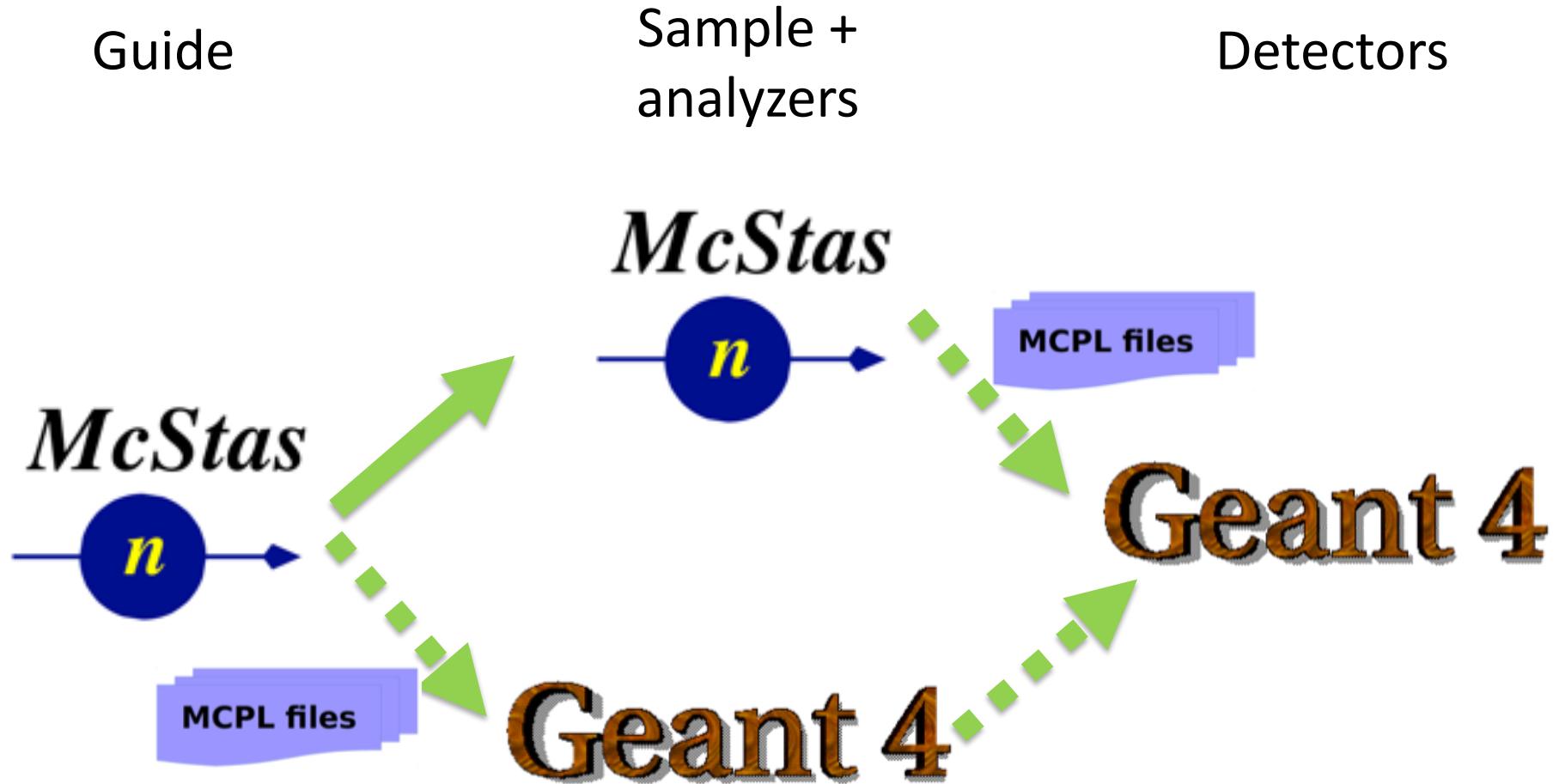
# Simulation Tools - Options



# Simulation Tools - Options



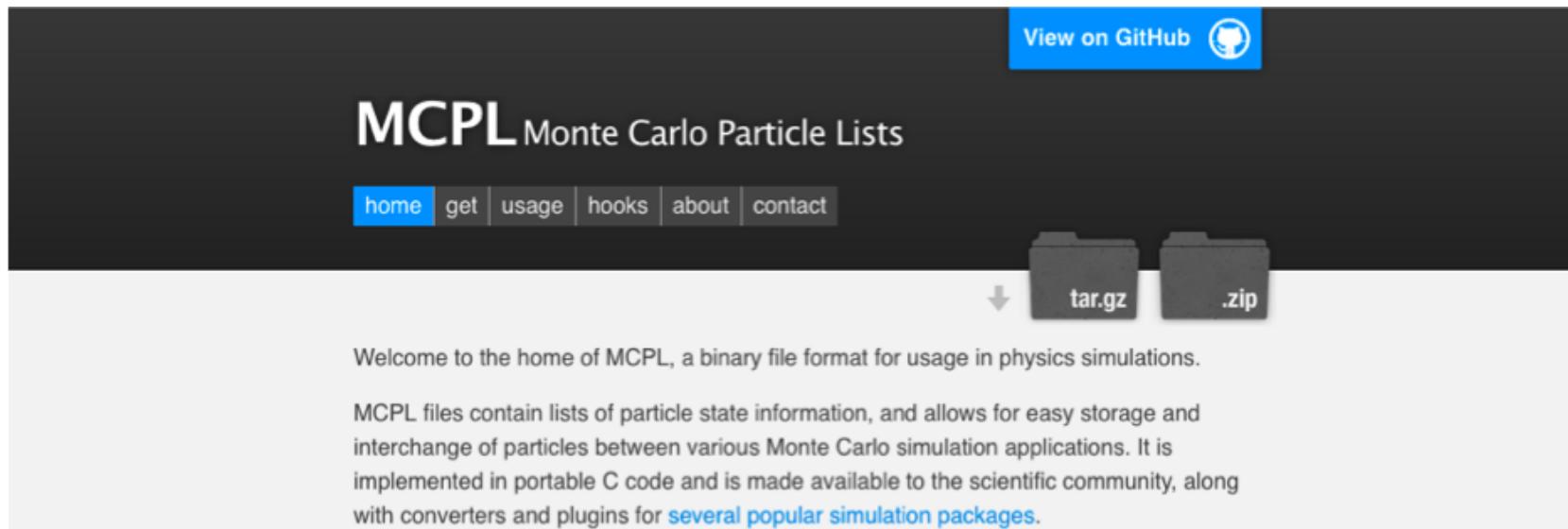
# Simulation Tools - Options



# Monte Carlo Simulation: MCPL



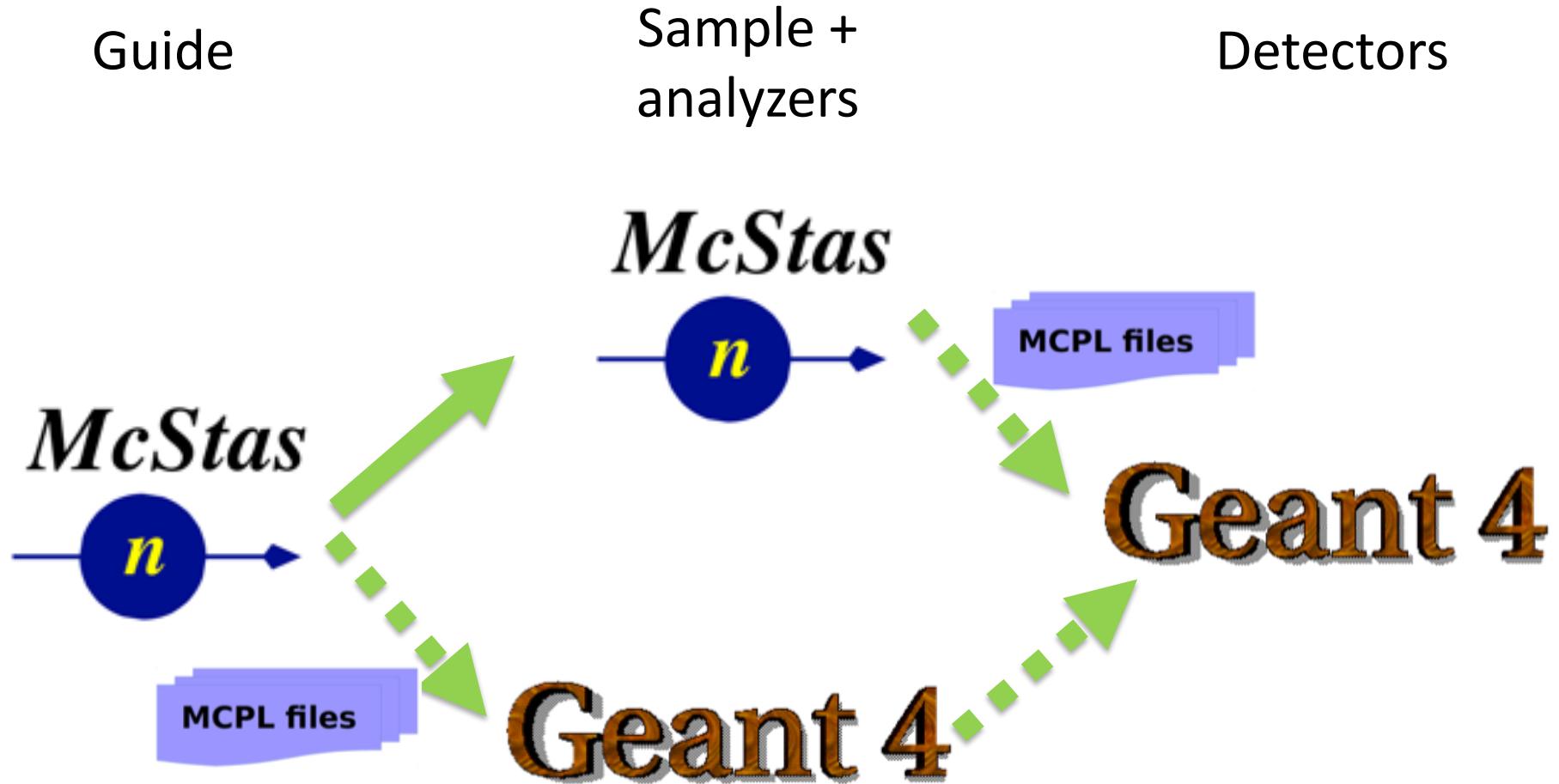
- Monte Carlo Particle List
- Binary format
- Open source
- Compatible MC tools
  - McStas
  - McXtrace
  - Geant4
  - MCNP6, MCNPX



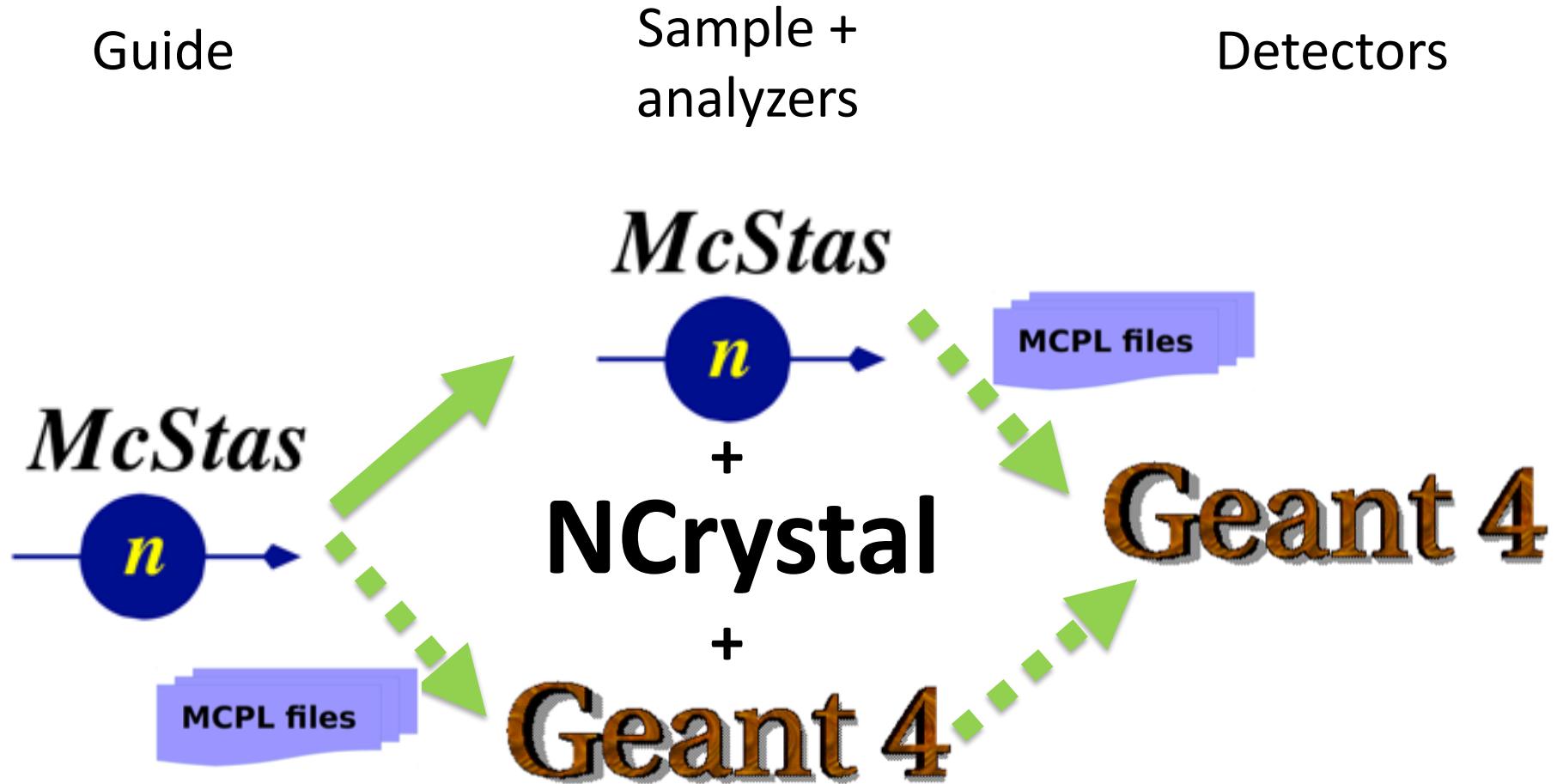
The screenshot shows the GitHub page for MCPL. At the top right is a blue button labeled "View on GitHub" with a GitHub icon. Below it, the title "MCPL Monte Carlo Particle Lists" is displayed in large white font. Underneath the title is a navigation bar with links: "home" (highlighted in blue), "get", "usage", "hooks", "about", and "contact". To the right of the navigation bar are two download icons: a folder labeled "tar.gz" and a folder labeled ".zip". A downward arrow is positioned between the two files. Below the navigation bar, a welcome message reads: "Welcome to the home of MCPL, a binary file format for usage in physics simulations." A detailed description follows: "MCPL files contain lists of particle state information, and allows for easy storage and interchange of particles between various Monte Carlo simulation applications. It is implemented in portable C code and is made available to the scientific community, along with converters and plugins for several popular simulation packages." The URL "Source: <https://mctools.github.io/mcpl/>" is at the bottom right of the page.

Source: <https://mctools.github.io/mcpl/>

# Simulation Tools - Options



# Simulation Tools - Options



# Simulation Tools: NCrystal



- Library + tools for thermal neutron transport in crystals
- Cross-platform, open source, v0.9.4
- Multiple interfaces (Geant4, McStas, ...), validated results
- Collaboration:
  - Xiao Xiao Cai (DTU, ESS)
  - Thomas Kittelmann (ESS)
- Supported by:
  - BrightnESS (No 676548)

A screenshot of the GitHub repository page for mctools/ncrystal. The top navigation bar shows tabs for 'This repository' (selected), 'Search', 'Pull requests', 'Issues', 'Marketplace', and 'Explore'. On the right, there are buttons for 'Watch' (2), 'Star' (2), and 'Fork' (1). Below the header, the repository name 'mctools / ncrystal' is displayed, along with links for 'Code', 'Issues 3', 'Pull requests 0', 'Projects 0', 'Wiki' (selected), and 'Insights'. The main content area is titled 'Home' and shows a message from Thomas Kittelmann edited on Aug 31, 2017. A summary of the repository's purpose and features is provided, followed by a 'Pages 8' section and a sidebar with links to 'Home', 'Get NCrystal', and 'Using NCrystal'.

Thomas Kittelmann edited this page on Aug 31, 2017 · 6 revisions

NCrystal : a library for thermal neutron transport in crystals

NCrystal is a library and associated tools which enables calculations for Monte Carlo simulations of thermal neutrons in crystals, focusing initially on scattering in single-crystals or polycrystalline materials and powders, including both coherent elastic (Bragg) diffraction and various models for inelastic scattering on phonons. Written in C++, interfaces and

Pages 8

Home  
Get NCrystal  
Using NCrystal

# Simulation Tools: NCrystal



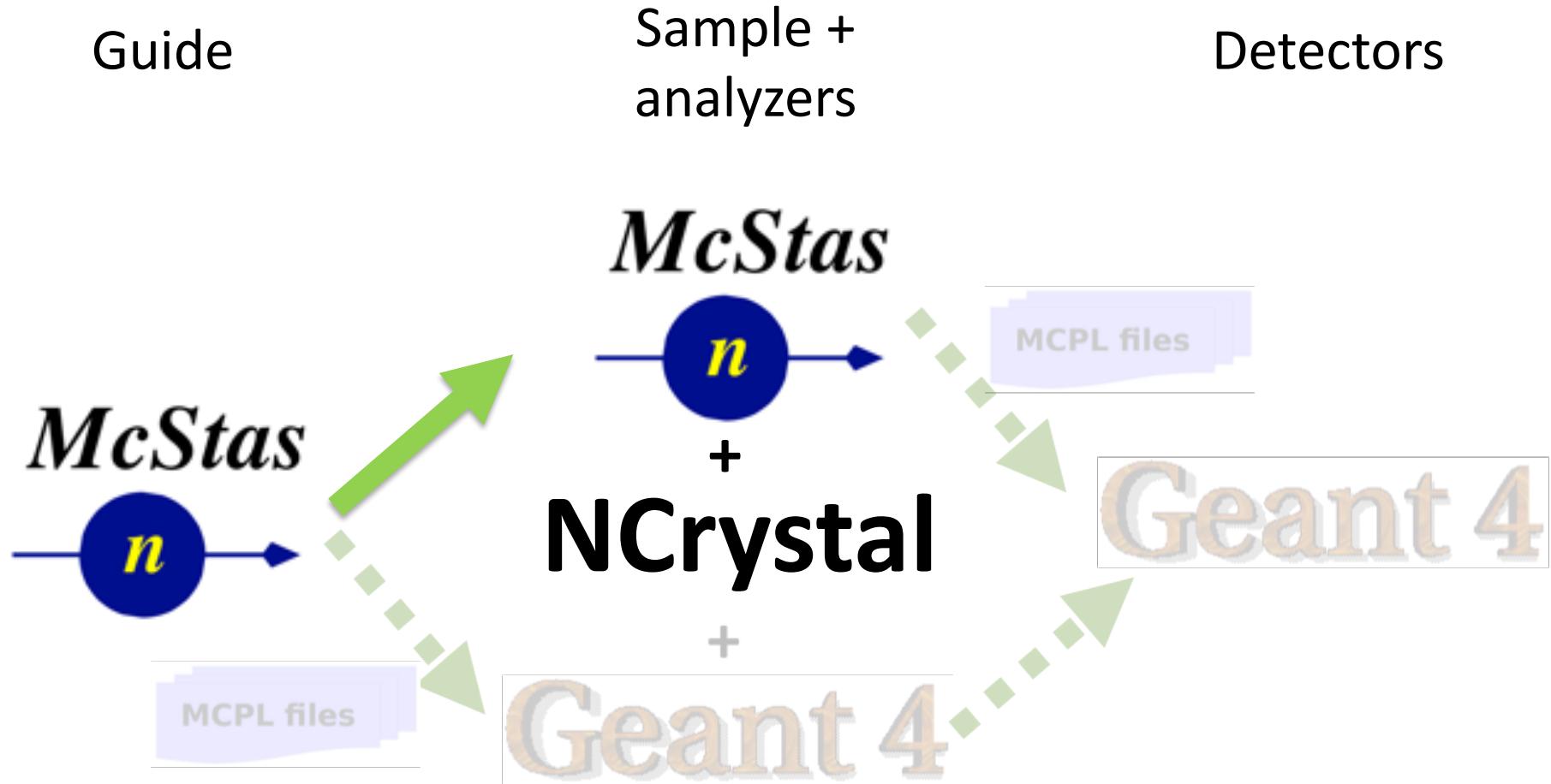
- Enables Monte Carlo simulation of neutrons in crystals
- Single-crystals
- Polycrystalline/powder materials
- Coherent elastic (Bragg) diffraction
- Includes "background" (inelastic/incoherent)
  - harmonic approximation
  - incoherent approximation
  - Debye approximation

# Simulation Tools: NCrystal



- Written in C++
- Direct usage from C, C++, or Python code
- Command-line tools
- **Components available for McStas and Geant4**

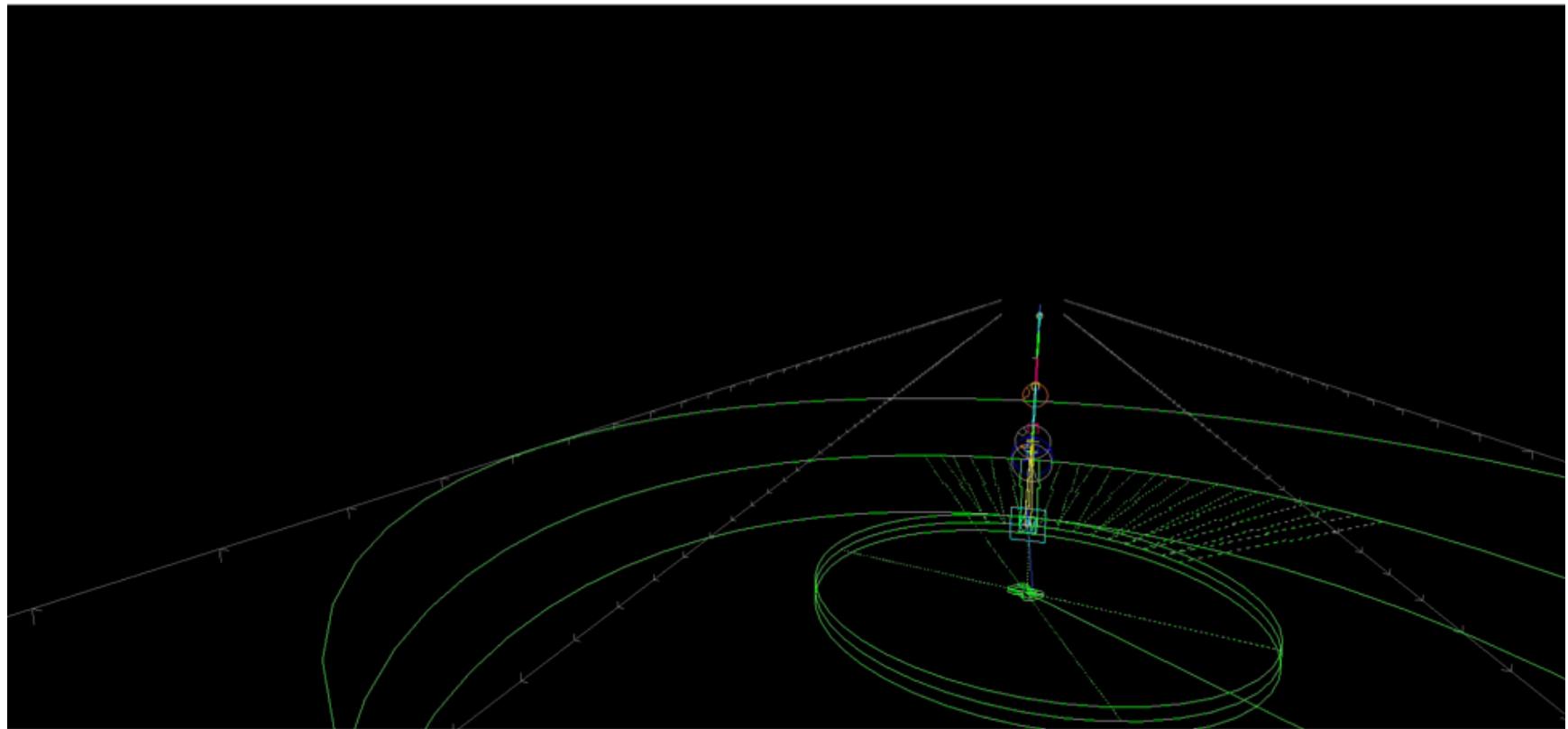
# Simulation Tools - Options



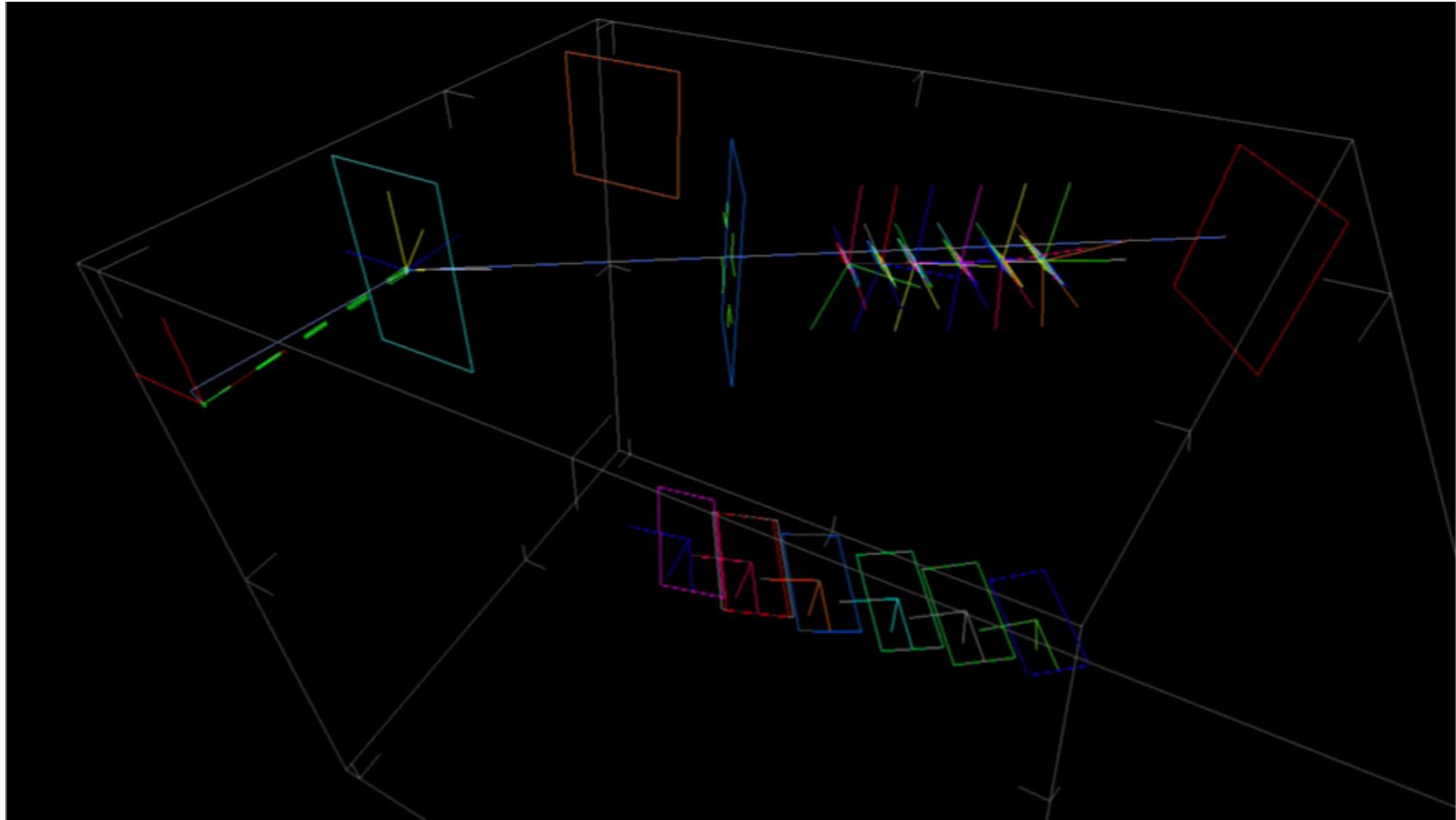
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# McStas Model – Full Instrument



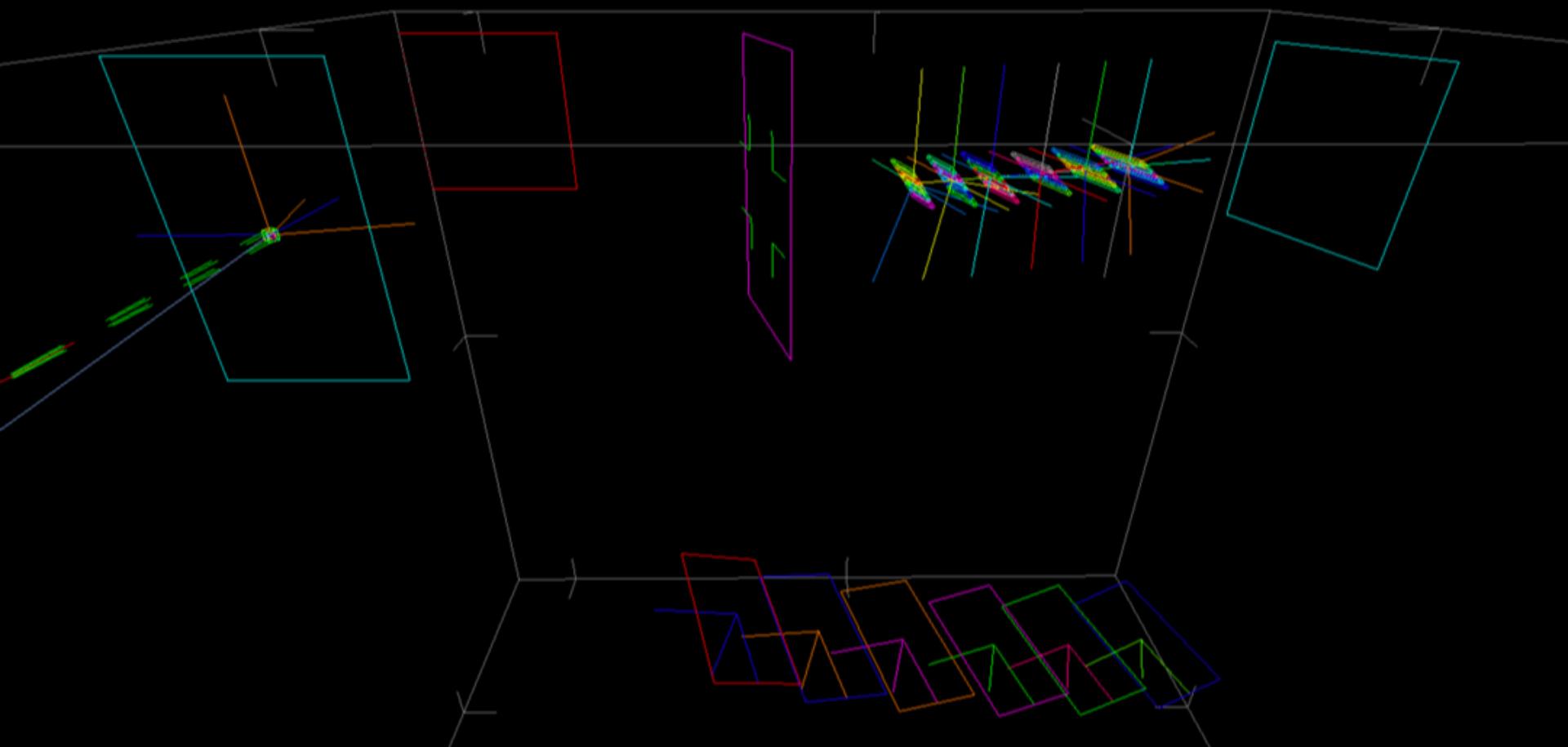
# McStas Model – Analyzer-Detector system



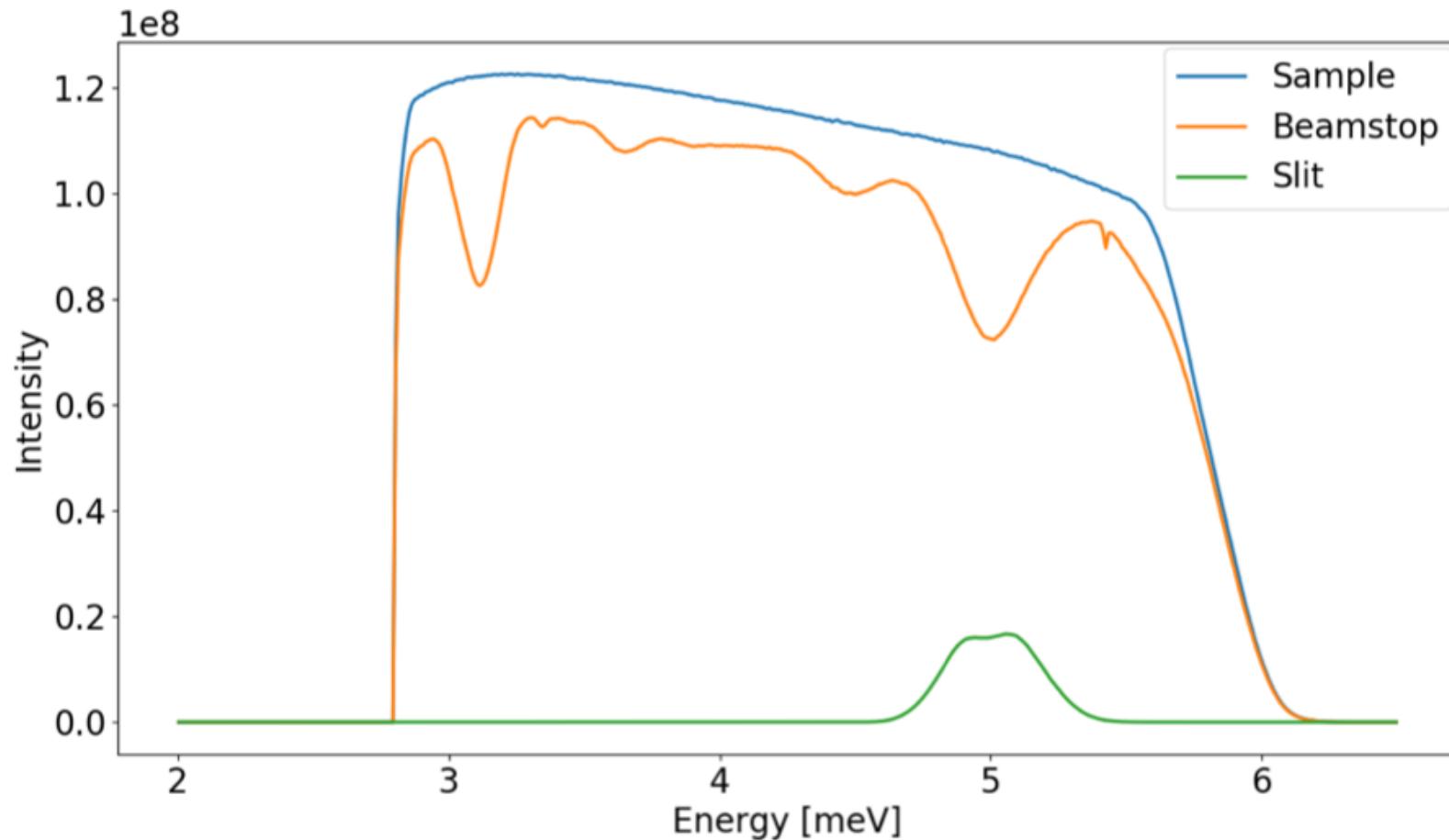
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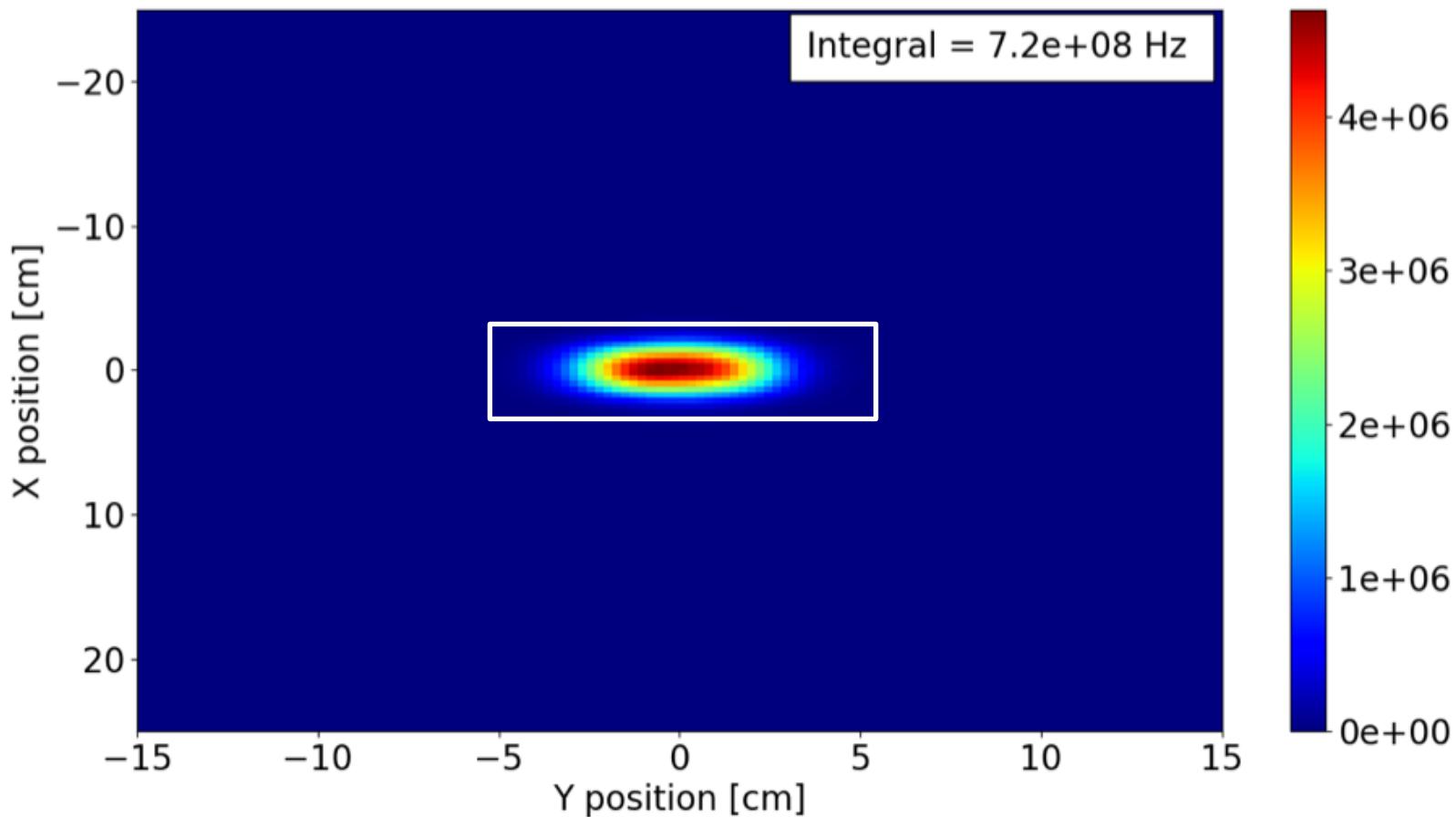
# TODO



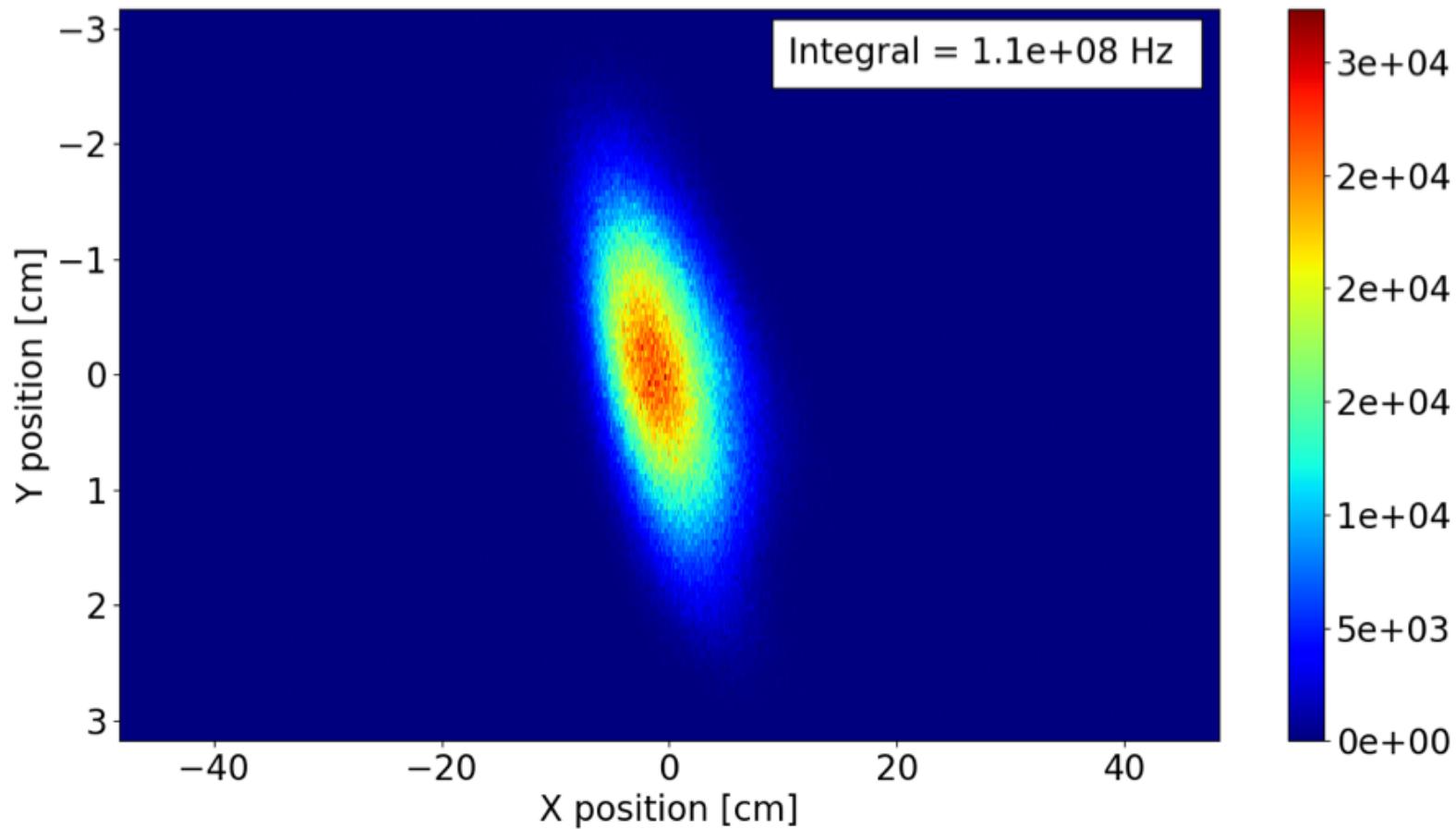
# Change of energy spectrum on sample



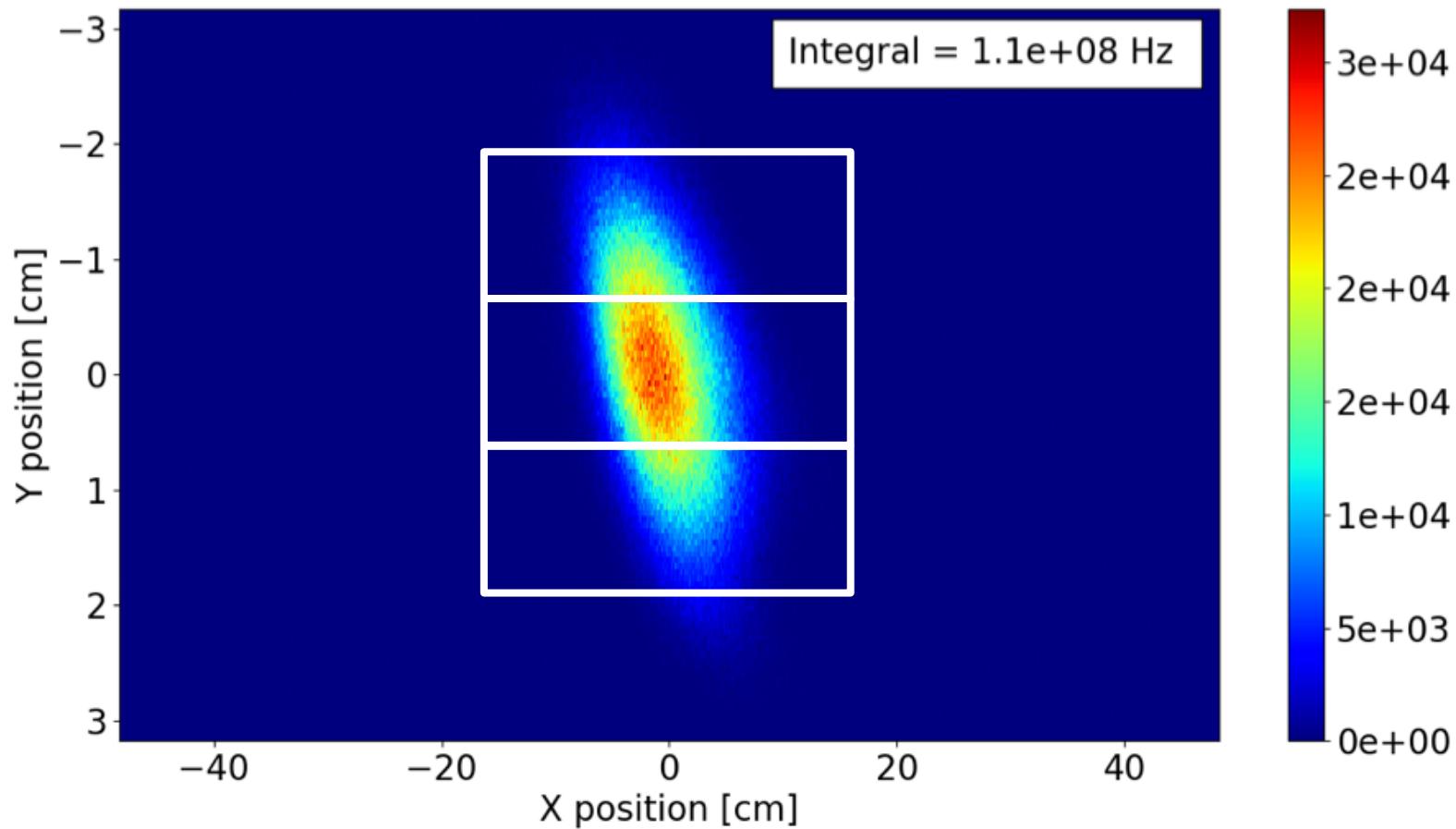
# Position on slit



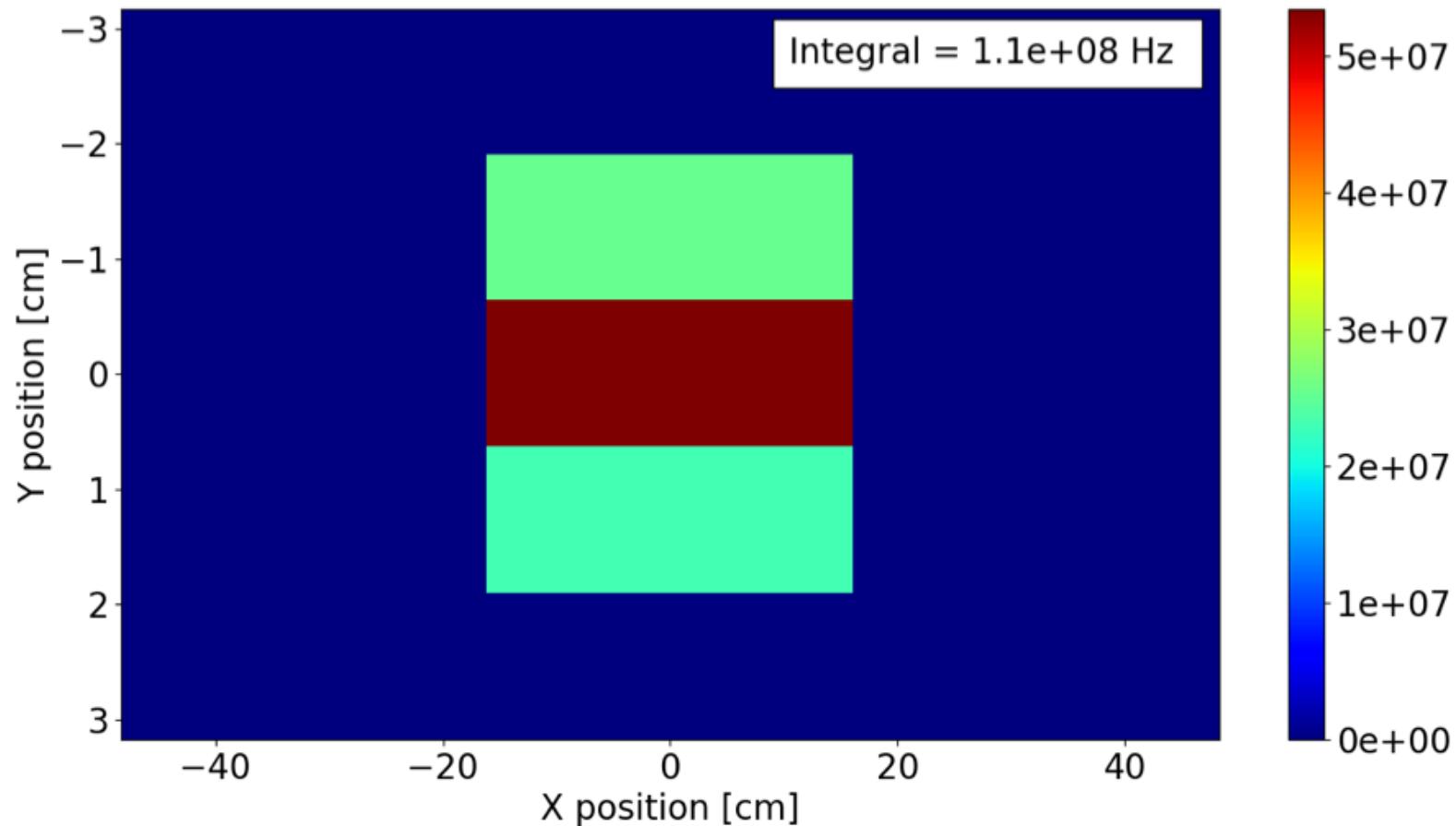
# Position on detector



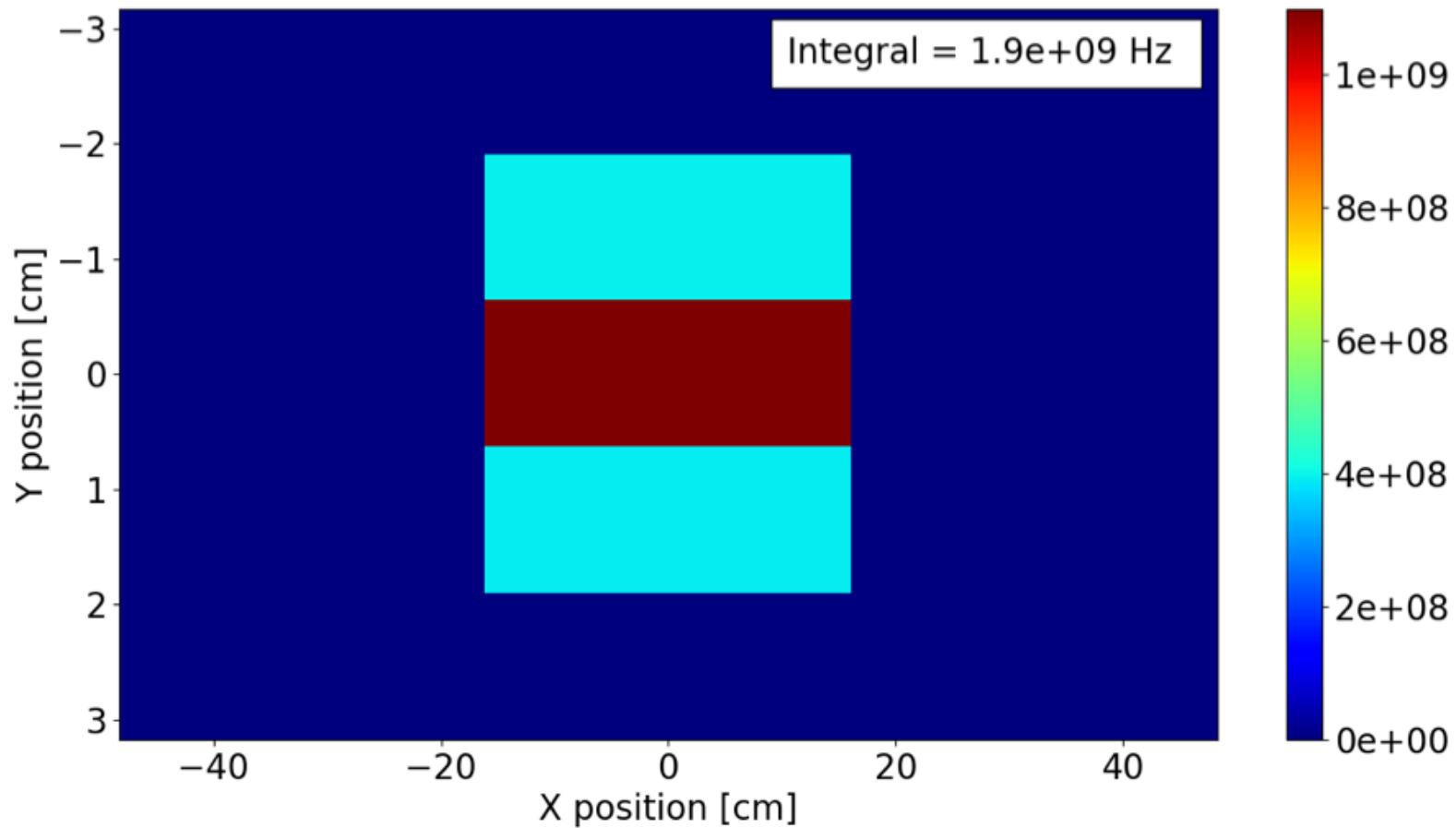
# Position on detector



# Time averaged incident rate



# Peak instantaneous incident rate



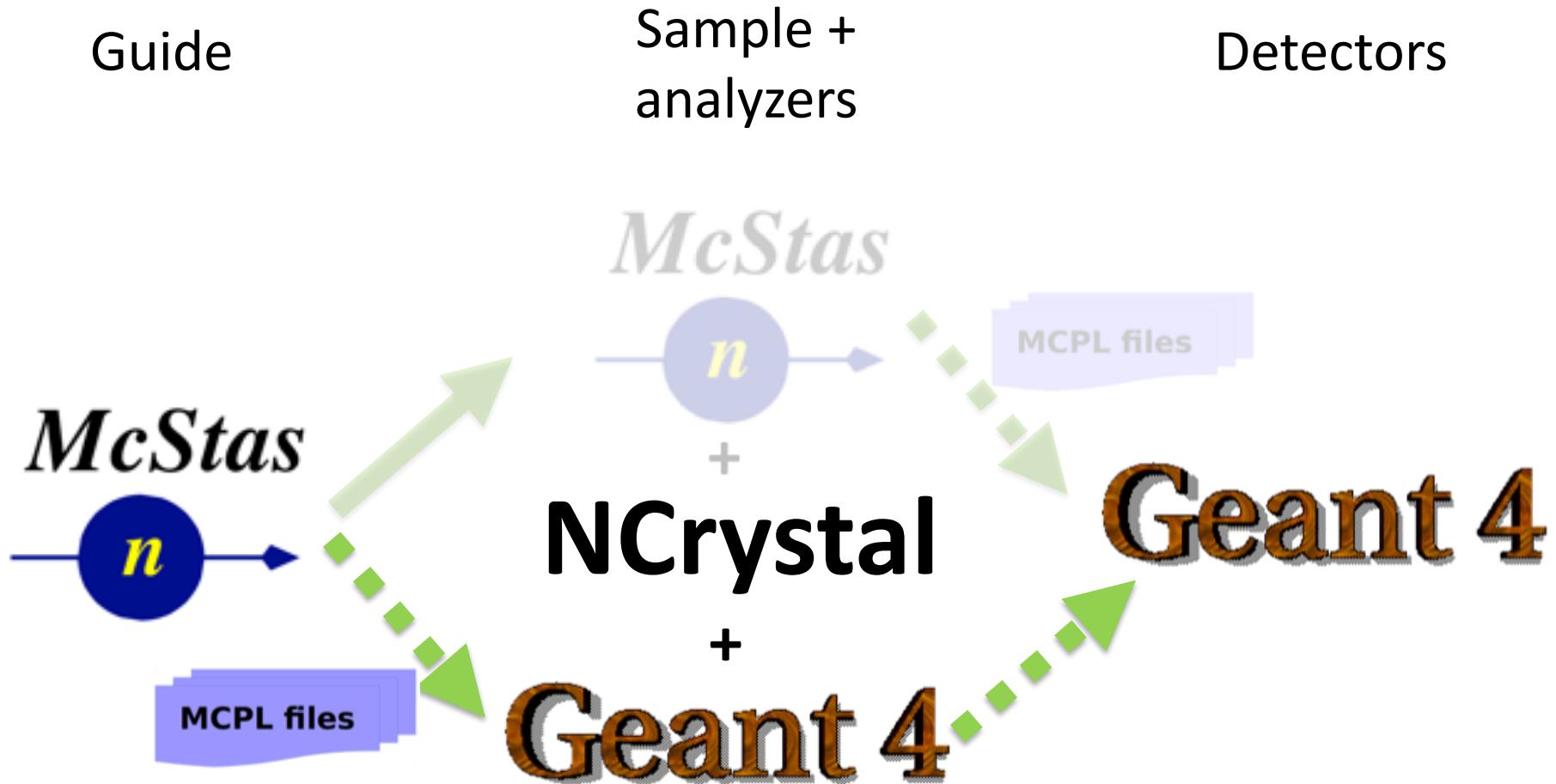
# Preliminary results

- Parameters:
  - Sample:  $\text{Y}_2\text{O}_3$  single-crystal,  $hkl=2,-2,-2$  ( $d_{hkl} = 3.0724 \text{ \AA}$ )  
size =  $(1.5 \text{ cm})^3$ , mosaicity = 60 arcmin
  - Analyzer: thickness = 2 mm, mosaicity = 10 arcmin
  - Source power = 5 MW
  - PSC opening time = 5 ms (full ESS pulse)
- Time averaged incident rate on one He tube: **5e7 Hz**
- Peak instantaneous incident rate on one Tube: **1e9 Hz**

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# Cross-check and Detector simulation

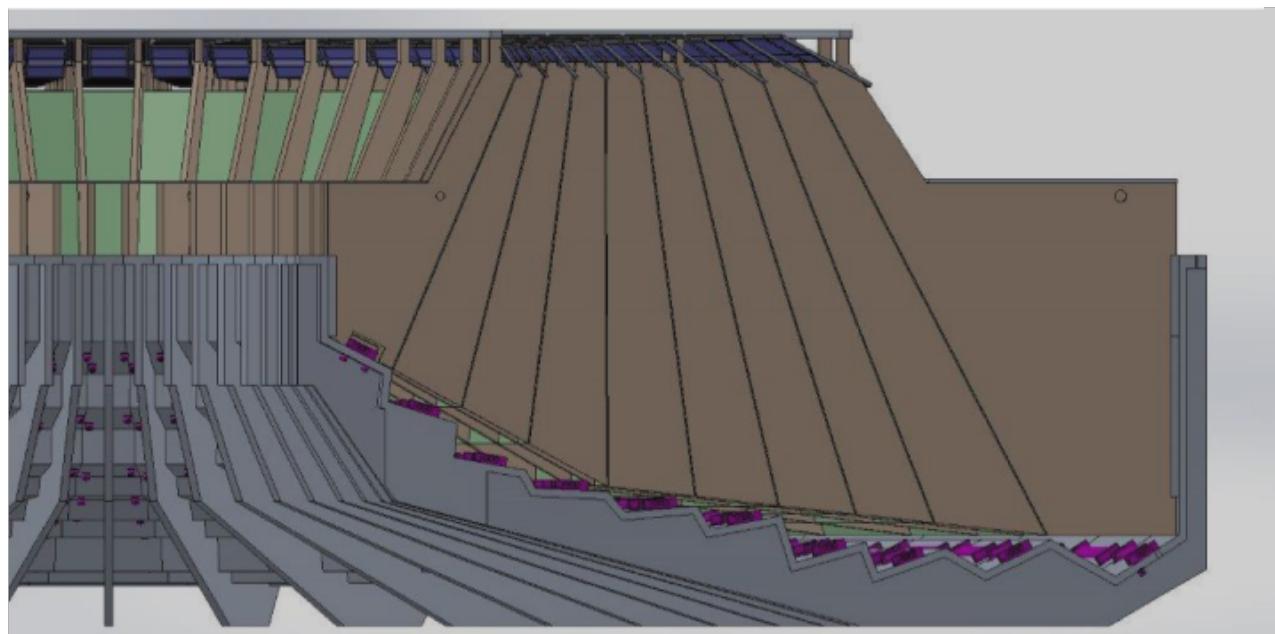
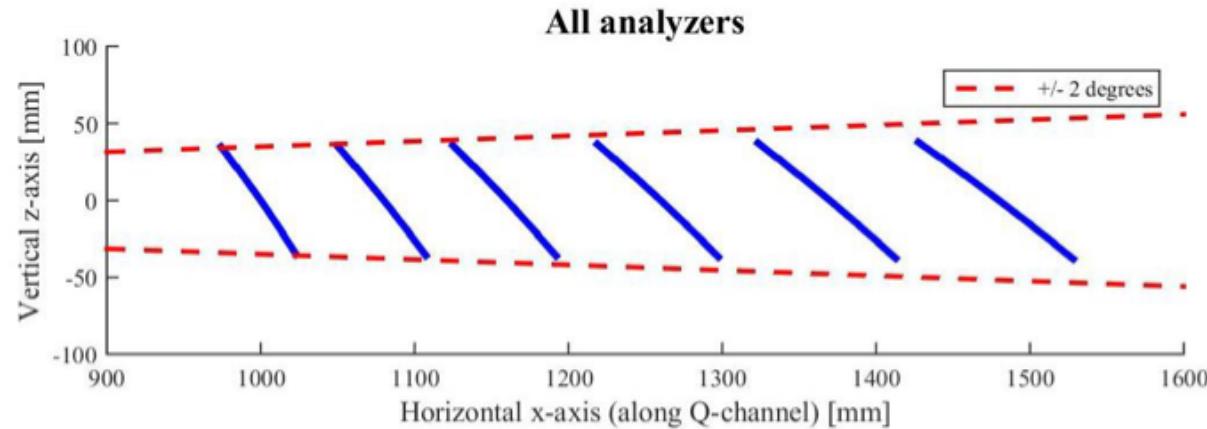


# Acknowledgments

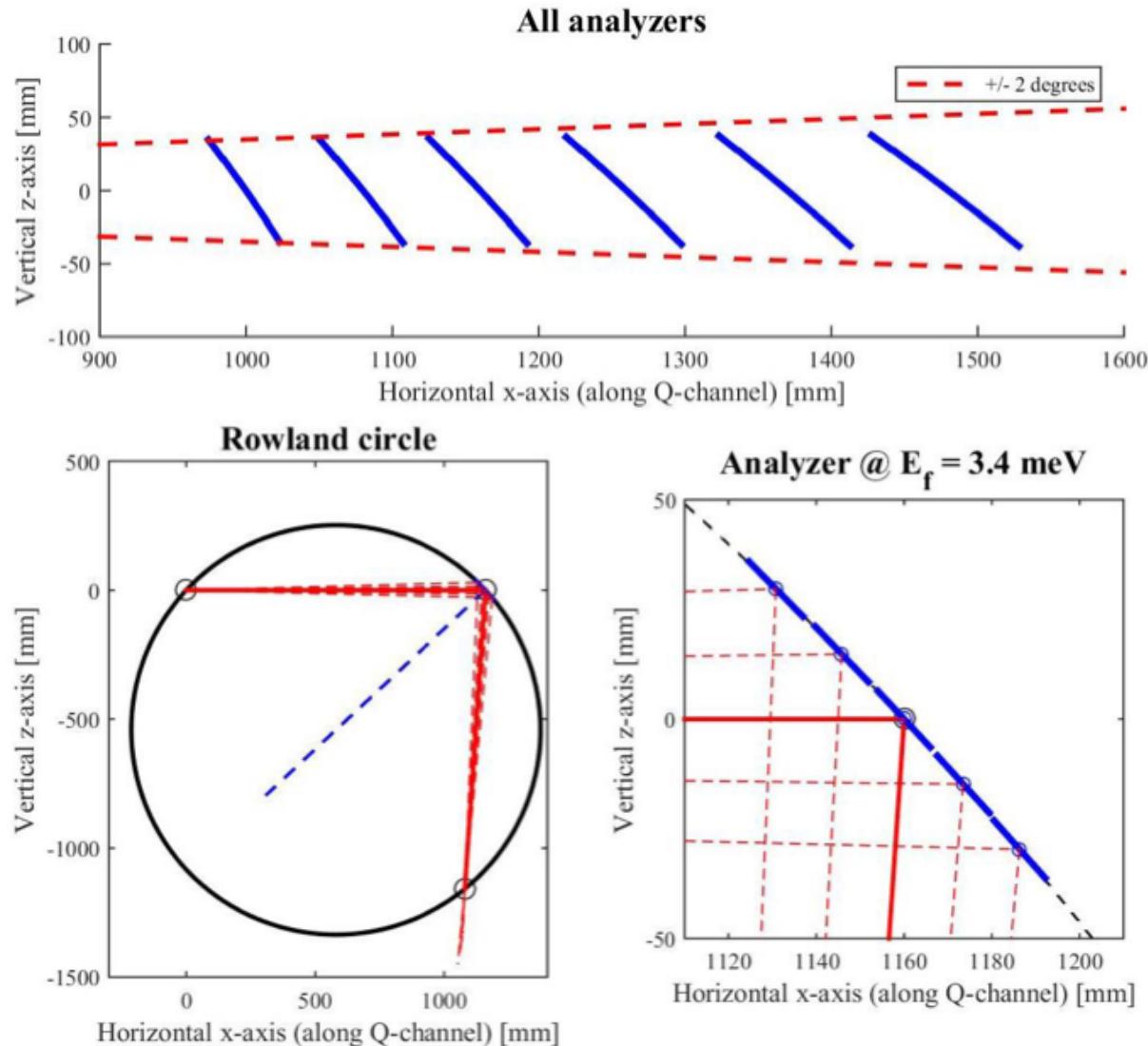
- Rasmus Toft-Petersen, Fatima Issa
- Thomas Kittelmann, Xiao Xiao Cai, Peter Willendrup
- Kalliopi Kanaki, Richard Hall-Wilton
- Data Management&Software Centre (DMSC)

Thank you for your  
attention!

# Secondary spectrometer tank - Analyzers

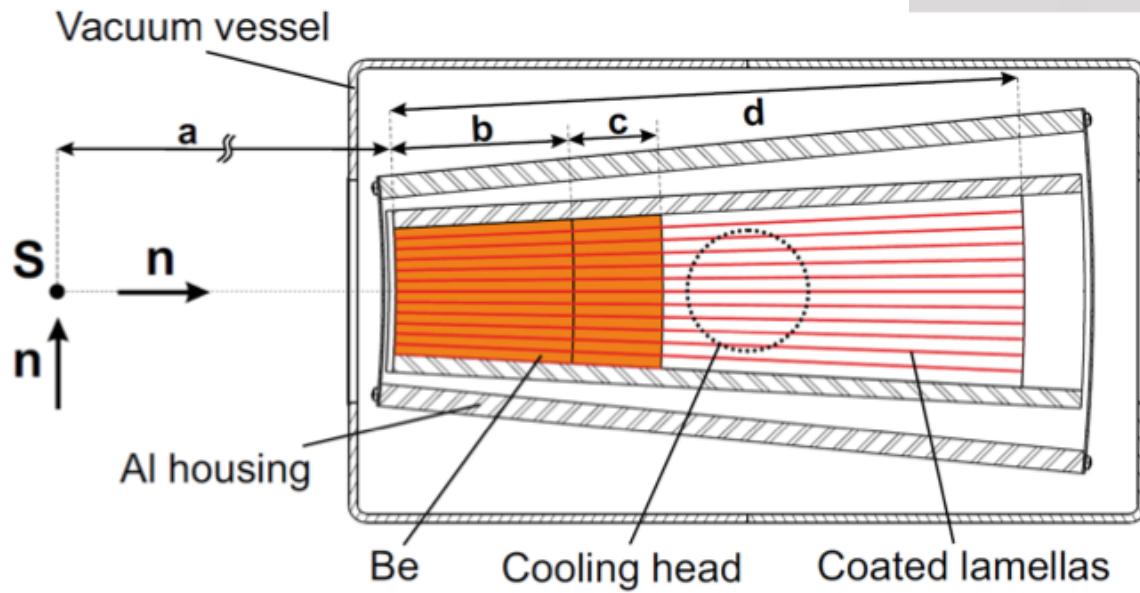
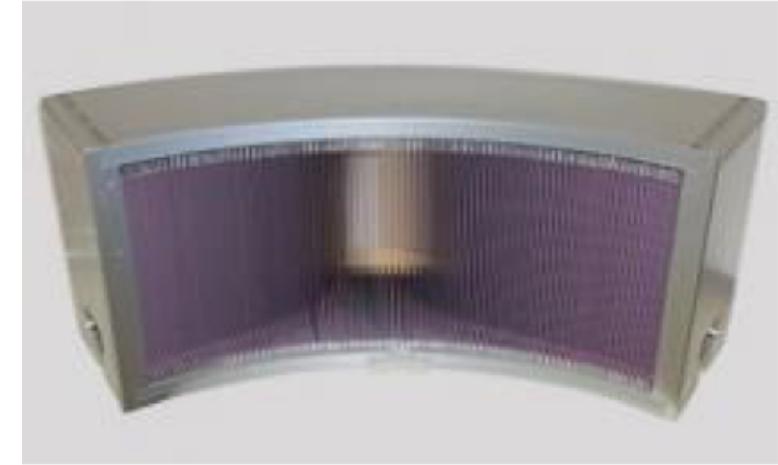


# Secondary spectrometer tank - Analyzers



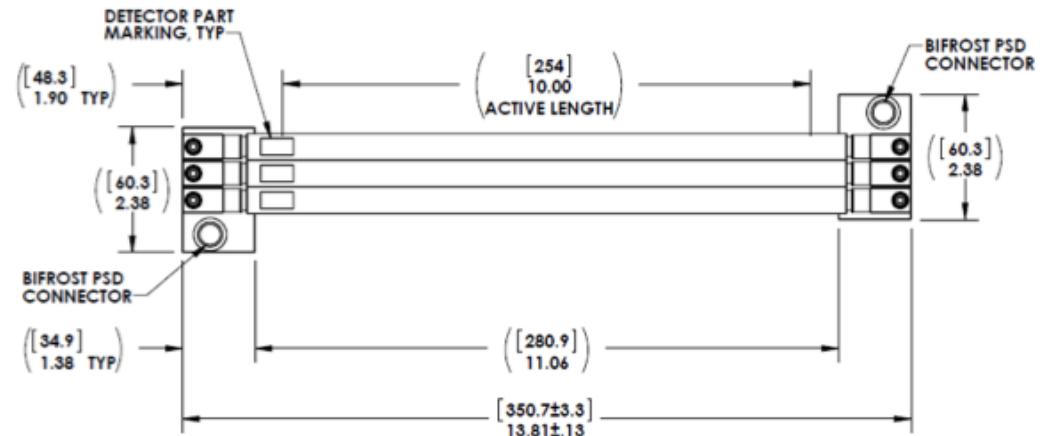
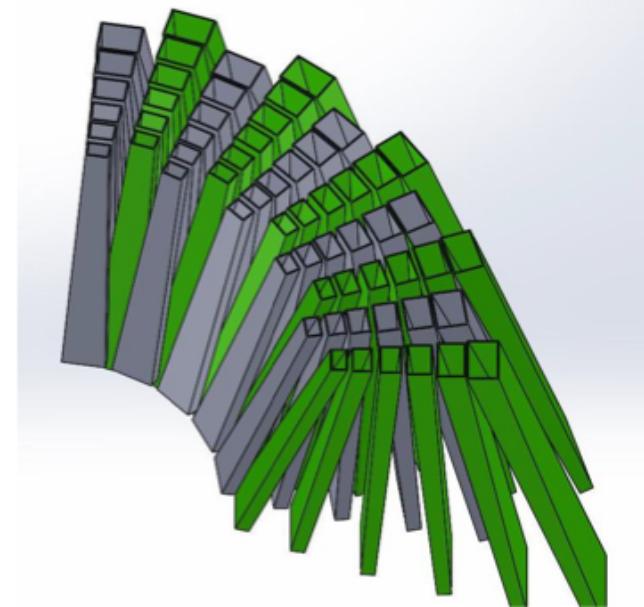
# Scattering Characterization System

- Filtering system
  - Beryllium filter
  - Radial collimator



# Secondary spectrometer tank - Detectors

- Crosstalk shielding
  - Prevent crosstalk between channels
- Detectors and electronics
  - He-3 tubes
  - Approx. 2x analyzer length



# Ncrystal - Data library and validation



```
NCMAT v1
#converted from the cif file of the entry 0014675 in the AMCSDB
#reference: Trucano P, Chen R, Nature, vol. 258, p. 136-137, 1975.
#Validated against EXFOR subentries 11359002,21149003 and 13761003
#(see https://github.com/mctools/ncrystal/wiki/Data-library)
#It is suitable to model large mosaicity graphite monochromators or analysers.
@CELL
    lengths 2.464 2.464 6.711
    angles 90. 90. 120.
@SPACEGROUP
    194
@ATOMPOSITIONS
    C 0. 0. 0.25
    C 0. 0. 0.75
    C 0.333333333333 0.666666666667 0.25
    C 0.666666666667 0.333333333333 0.75
@DEBYETEMPERATURE
    C 730.950029766
```

# Ncrystal - Data library and validation

```

NCMAT v1
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#reference: Trucano P, Chen R, Nature, vol. 258, p. 136-137, 1975.
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@CELL
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@SPACEGROUP
    194
@ATOMPOSITIONS
    C 0. 0. 0.25
    C 0. 0. 0.75
    C 0.333333333333 0.666666666667 0.25
    C 0.666666666667 0.333333333333 0.75
@DEBYETEMPERATURE
    C 730.950029766

```

