

Detector rate estimate for the BIFROST instrument at ESS

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Péter Zagyvai^{1,3}, Jonas Okkels Birk, Martin Olsen⁴, Richard Hall-Wilton^{2,5}

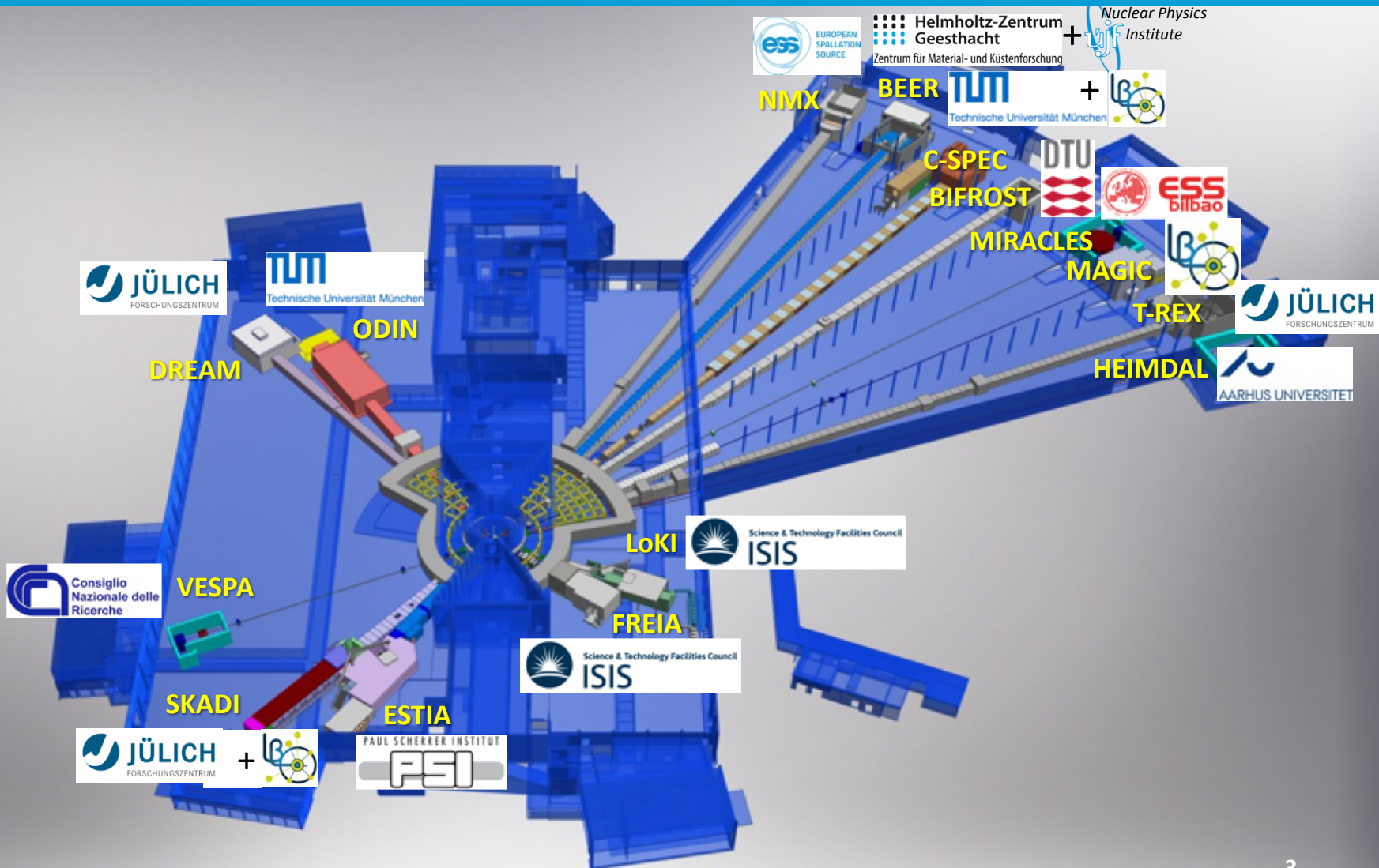
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HAS Centre for Energy Research
European Spallation Source ESS ERIC
BUTE Institute of Nuclear Techniques
Technical University of Denmark
Università degli Studi di Milano-Bicocca

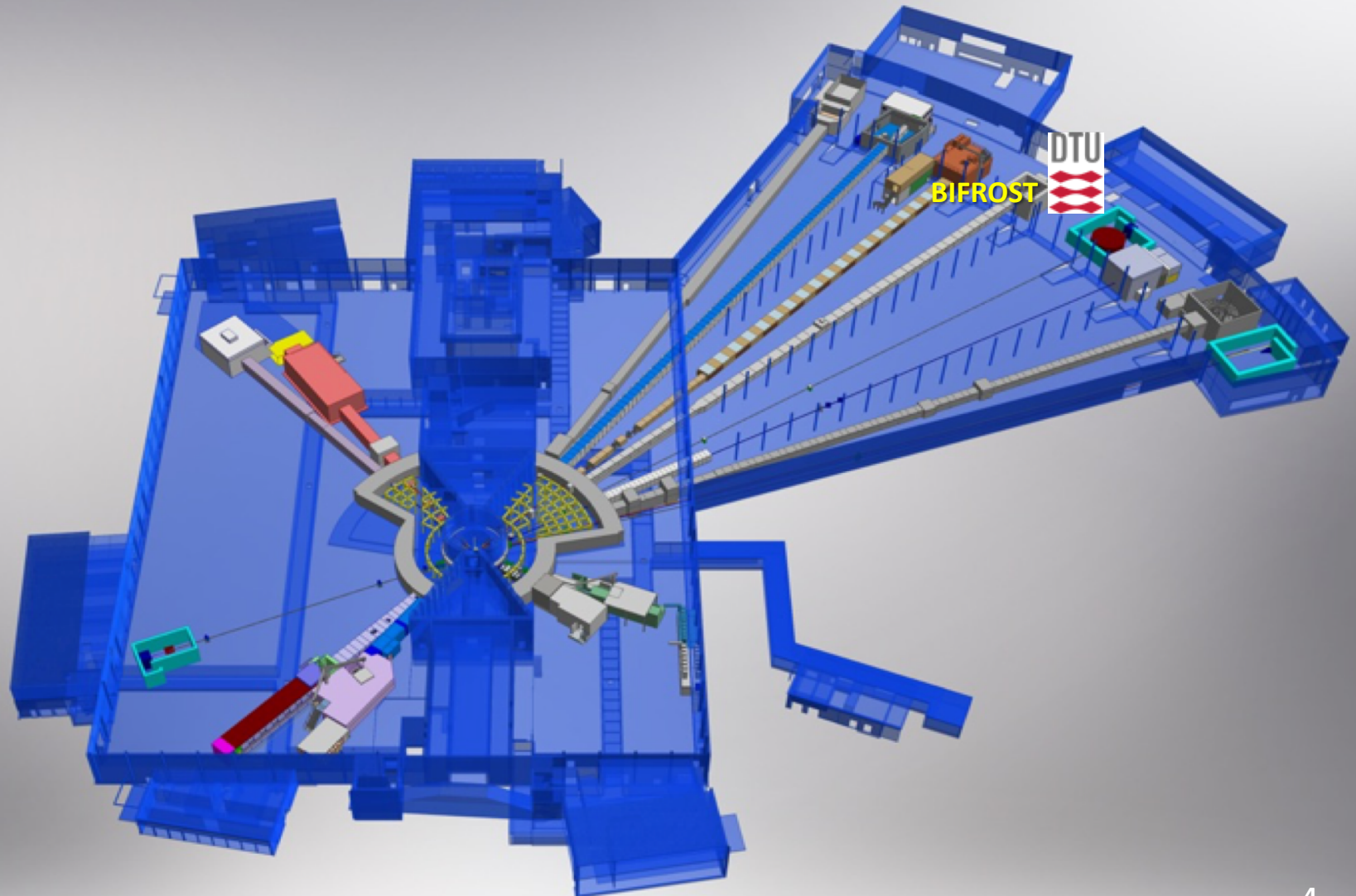
ICANS XXIII
Chattanooga, 17 October 2019

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

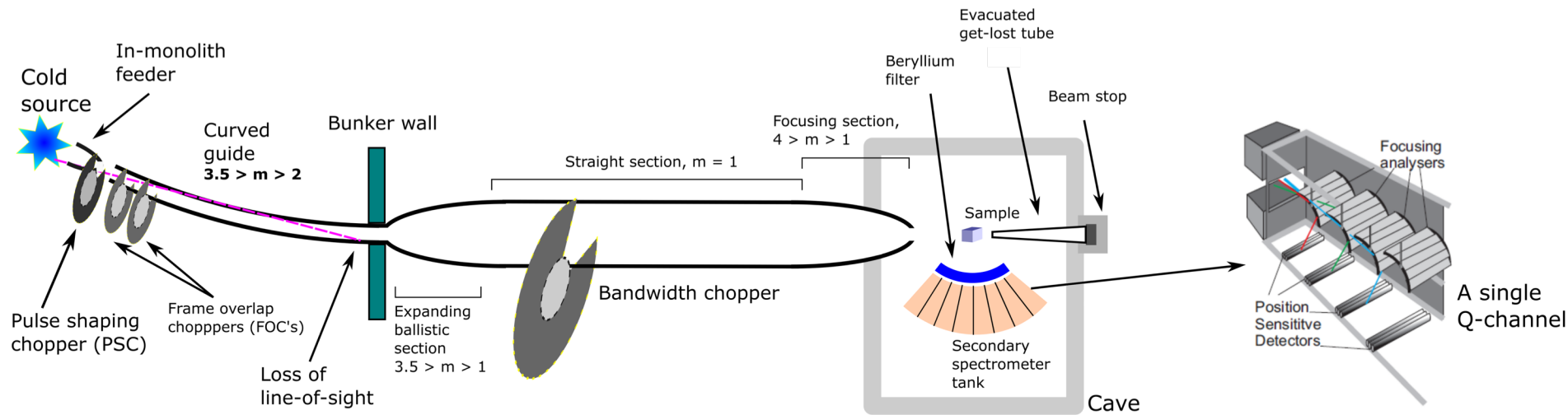
ESS - Instruments



Location of BIFROST

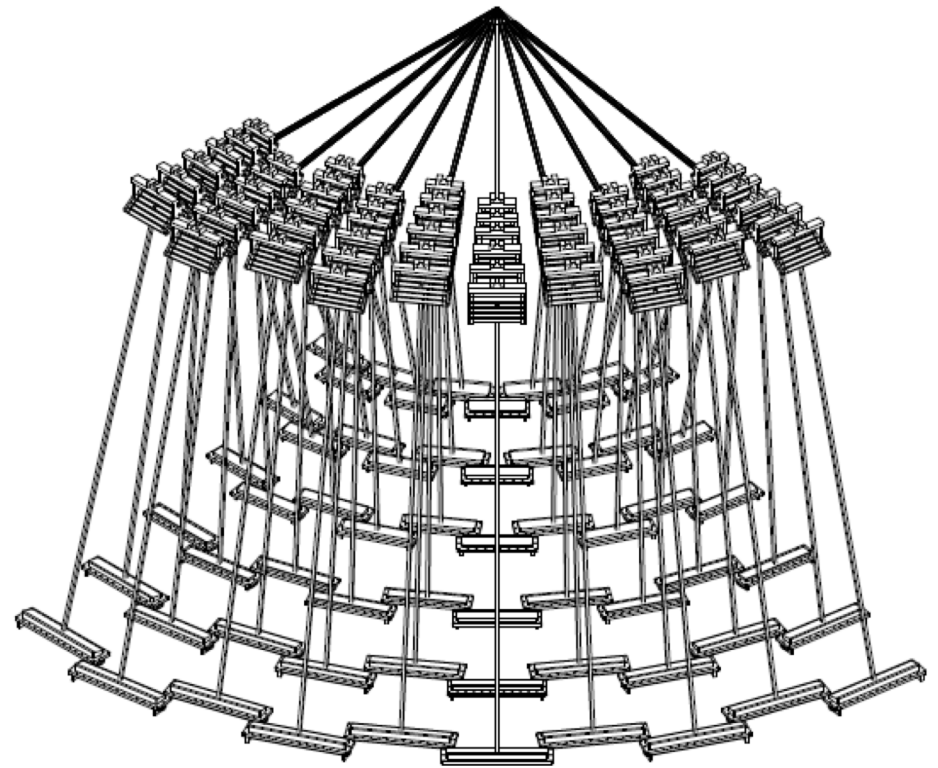
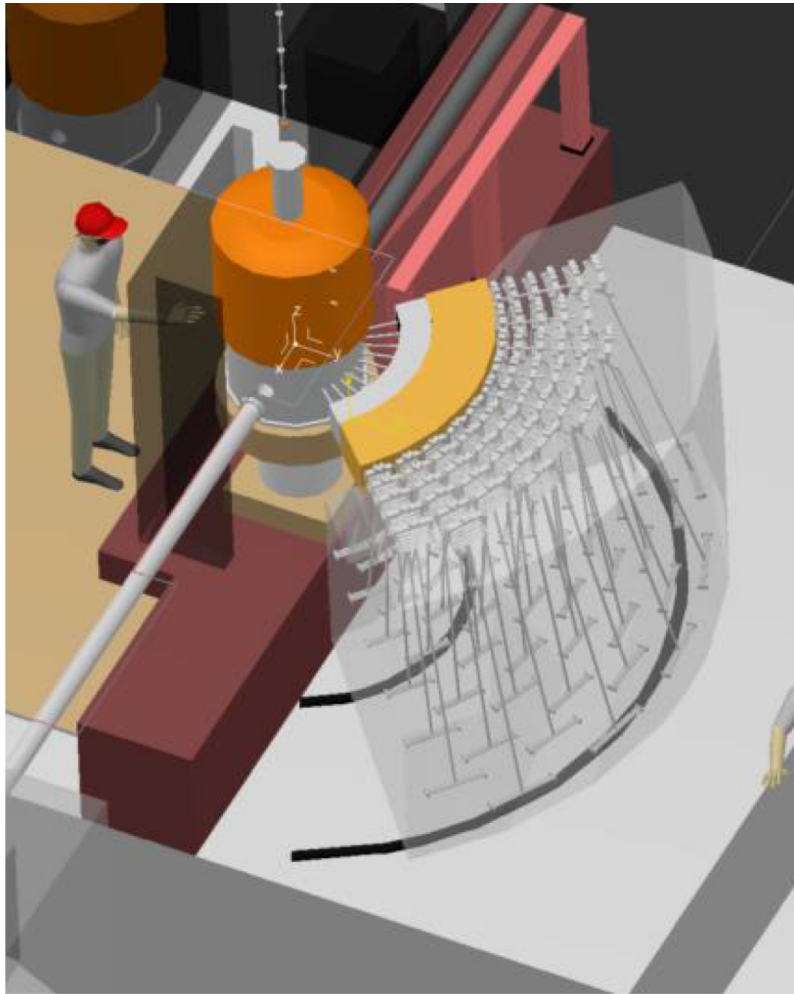


Bifrost instrument

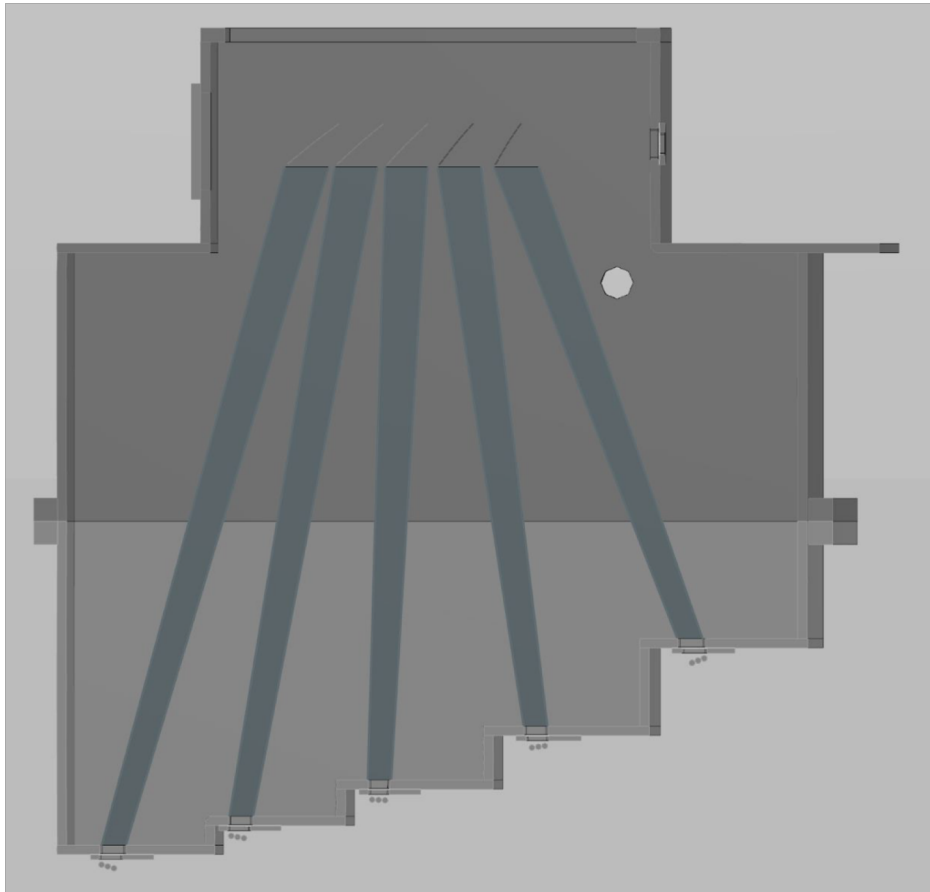


- High flux indirect geometry cold spectrometer
- Small sample (1 mm^3) in extreme environment
- Relatively simple beam transport and conditioning system
- Option to use full ESS pulse in low resolution mode

Scattering Characterization System



Scattering Characterization System



- **10^{10} n/s/cm²** flux on sample
- Detect weak inelastic signal
- Survive intense Bragg peak
- Important to define the incident detector rate

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Simulation Tools - Options

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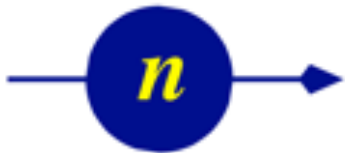
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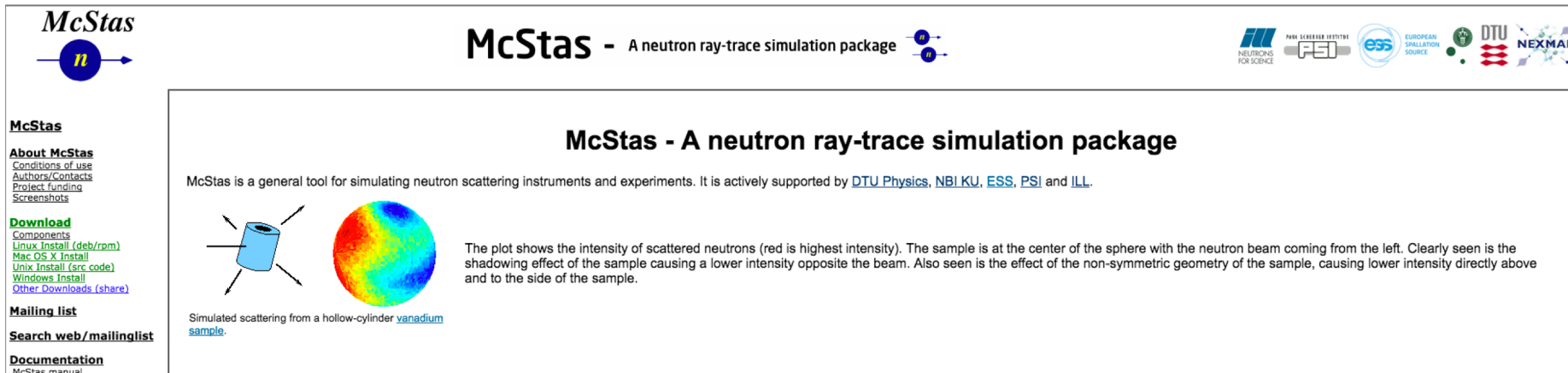
Detectors

McStas



Simulation Tools - McStas

- Simulation of neutron scattering instruments and experiments
 - Monte Carlo ray-trace algorithm
 - Cross-platform, open source
 - Version 2.5 (December, 2018)
- Collaboration:
 - DTU Physics
 - University of Copenhagen
 - Paul Scherrer Institute
 - Institut Laue-Langevin



The screenshot shows the McStas website. At the top left is the McStas logo, a blue circle with a white 'n' and a blue arrow pointing right. To its right is the text 'McStas - A neutron ray-trace simulation package' followed by a small logo of three blue circles. Further right are logos for 'INSTRUMENTS FOR SCIENCE', 'PSI', 'ESS', 'EUROPEAN SPALLATION SOURCE', 'DTU', and 'NEXMAP'. Below the header is a navigation menu with links: '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', and 'Other Downloads (share)'. Below the menu is a 'Mailing list' and 'Search web/ mailinglist' section. The main content area has the title 'McStas - A neutron ray-trace simulation package' and a paragraph: '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 of a hollow cylinder with a neutron beam entering from the left, and a corresponding 2D intensity plot of scattered neutrons. The plot shows a bright spot on the left and a shadowed region on the right. Below the plot is the text: '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.' At the bottom left of the main content area is the text: 'Simulated scattering from a hollow-cylinder [vanadium sample](#).'

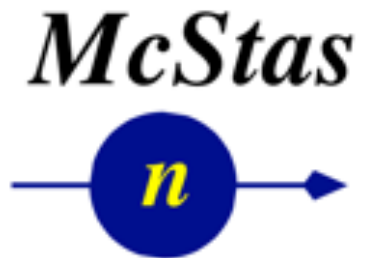
Source: <http://mcstas.org/>

Simulation Tools - Options

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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

Geant 4

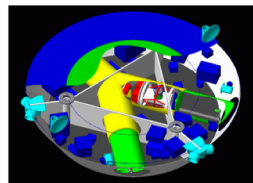
Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The two main reference papers for Geant4 are published in *Nuclear Instruments and Methods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

Applications



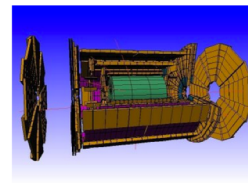
A sampling of applications, technology transfer and other uses of Geant4

User Support



Getting started, guides and information for users and developers

Publications



Validation of Geant4, results from experiments and publications

Collaboration



Who we are: collaborating institutions, members, organization and legal information

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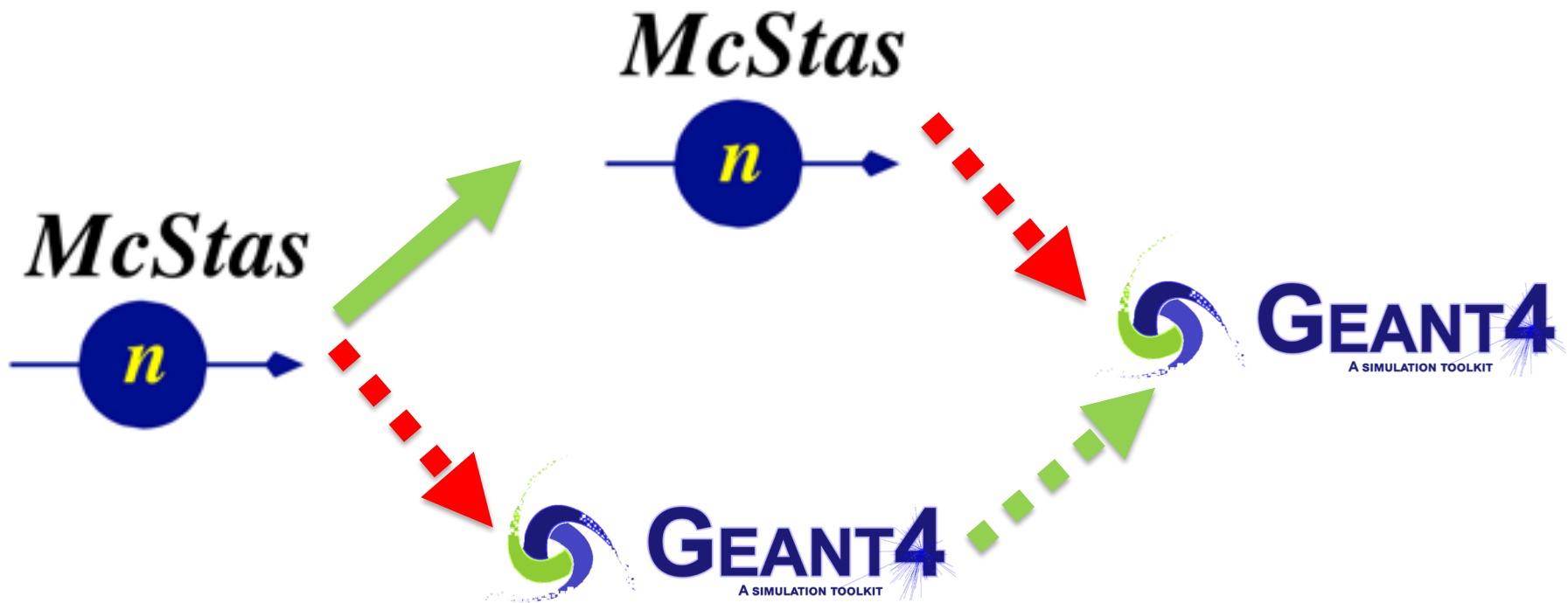


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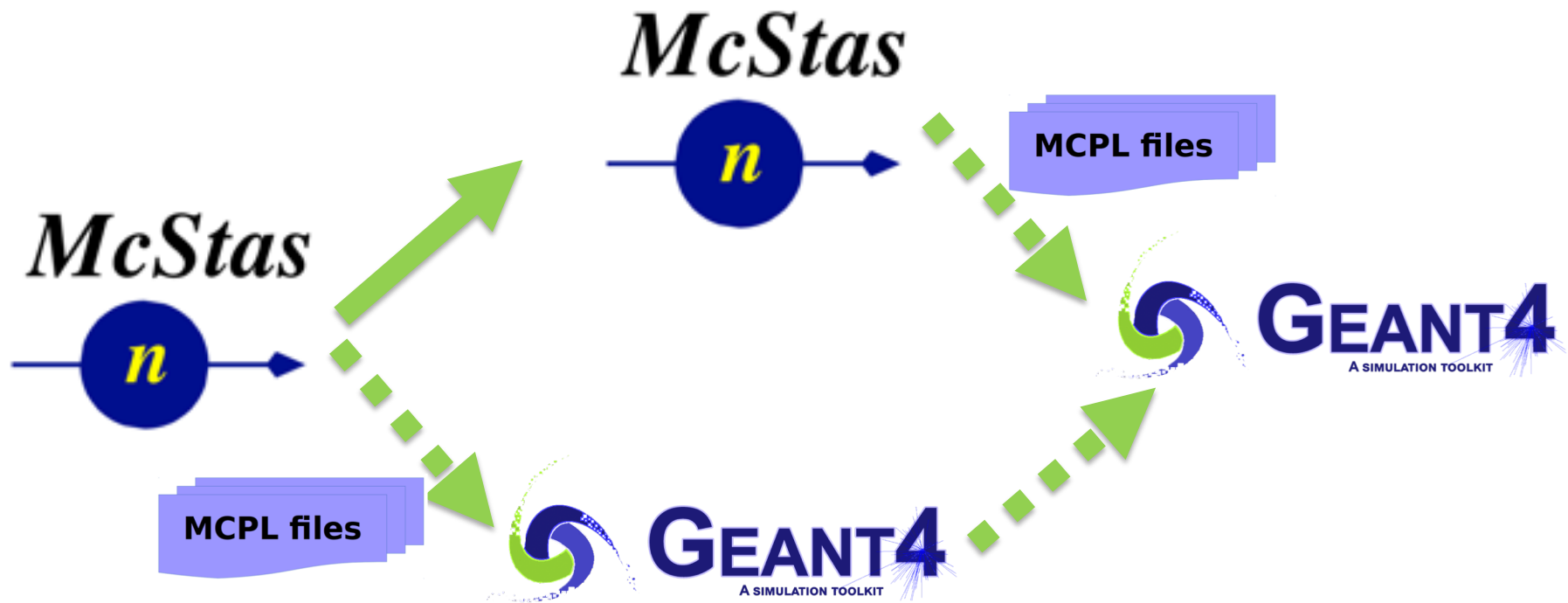


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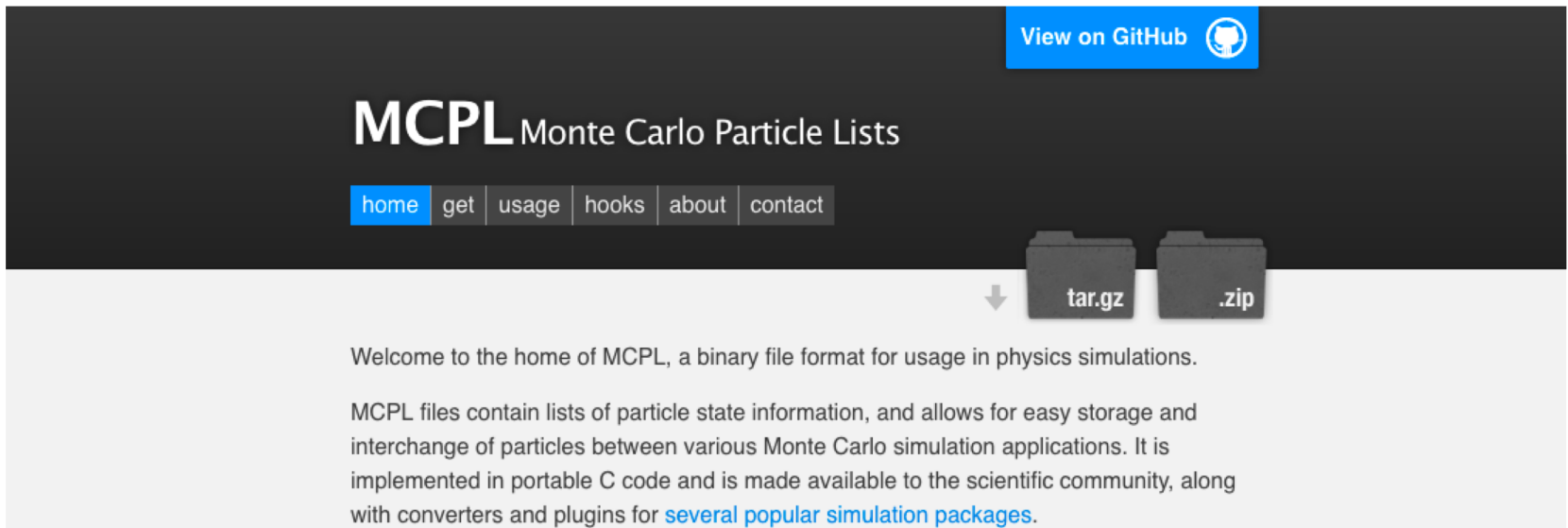
Sample +
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Monte Carlo Simulation: MCPL

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



The screenshot shows the homepage of the MCPL project. At the top right, there is a blue button labeled "View on GitHub" with the GitHub logo. The main heading is "MCPL Monte Carlo Particle Lists". Below the heading is a navigation menu with links for "home", "get", "usage", "hooks", "about", and "contact". The "home" link is highlighted. Below the navigation menu, there are two folder icons labeled "tar.gz" and ".zip" with a downward arrow pointing to them. The main content area contains a welcome message and a description of MCPL files.

View on GitHub 

MCPL Monte Carlo Particle Lists

[home](#) [get](#) [usage](#) [hooks](#) [about](#) [contact](#)

↓ [tar.gz](#) [.zip](#)

Welcome to the home of MCPL, a binary file format for usage in physics simulations.

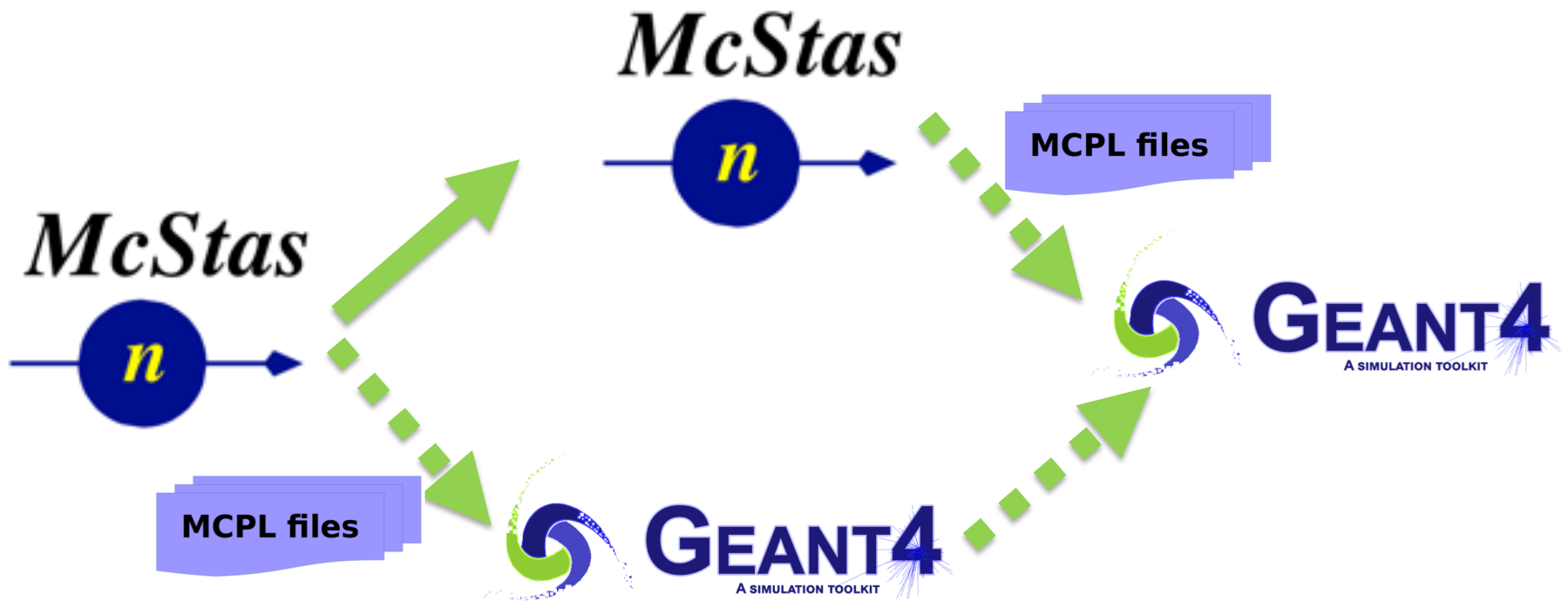
MCPL files contain lists of particle state information, and allows for easy storage and interchange of particles between various Monte Carlo simulation applications. It is implemented in portable C code and is made available to the scientific community, along with converters and plugins for [several popular simulation packages](#).

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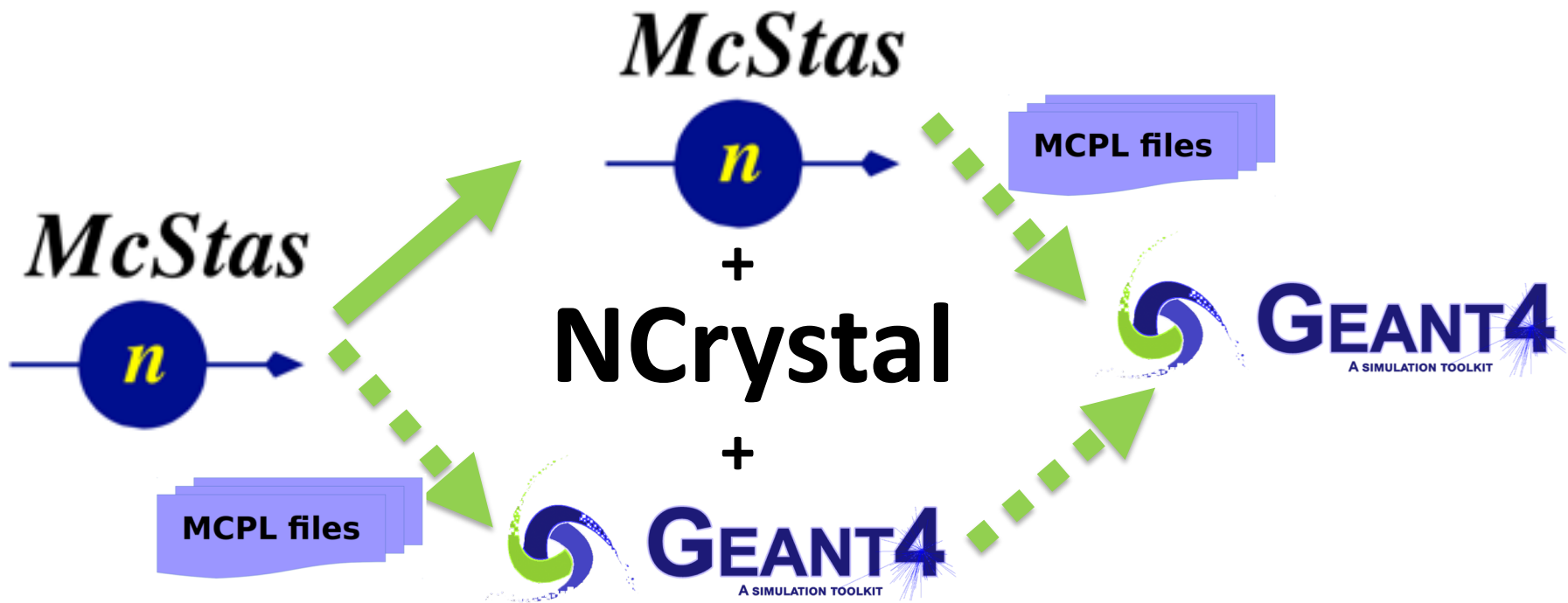


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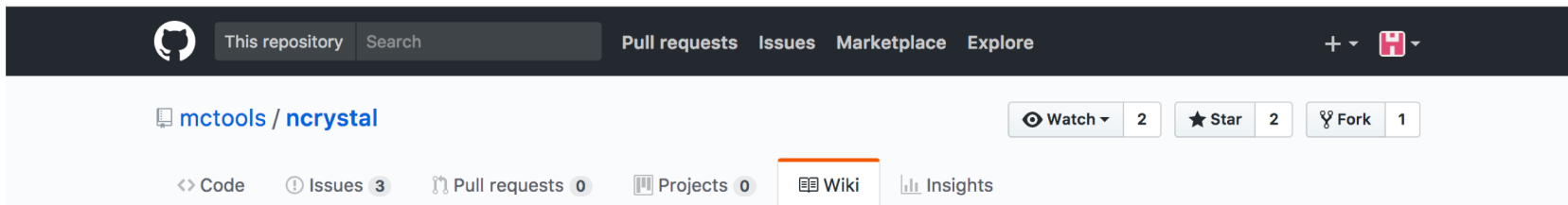
Sample +
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Detectors



Simulation Tools: NCrystal

- Library + tools for thermal neutron transport in crystals
- Cross-platform, open source, v1.0.0
- Multiple interfaces (Geant4, McStas, ...), validated results
- Collaboration:
 - Xiao Xiao Cai (CNCS)
 - Thomas Kittelmann (ESS)
- Supported by:
 - BrightnESS (No 676548)



The screenshot shows the GitHub repository page for `mctools/ncrystal`. The repository name is displayed in blue. Below the name, there are buttons for `Code`, `Issues` (3), `Pull requests` (0), `Projects` (0), `Wiki`, and `Insights`. On the right side, there are buttons for `Watch` (2), `Star` (2), and `Fork` (1). The top navigation bar includes `This repository`, `Search`, `Pull requests`, `Issues`, `Marketplace`, and `Explore`.

Home

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

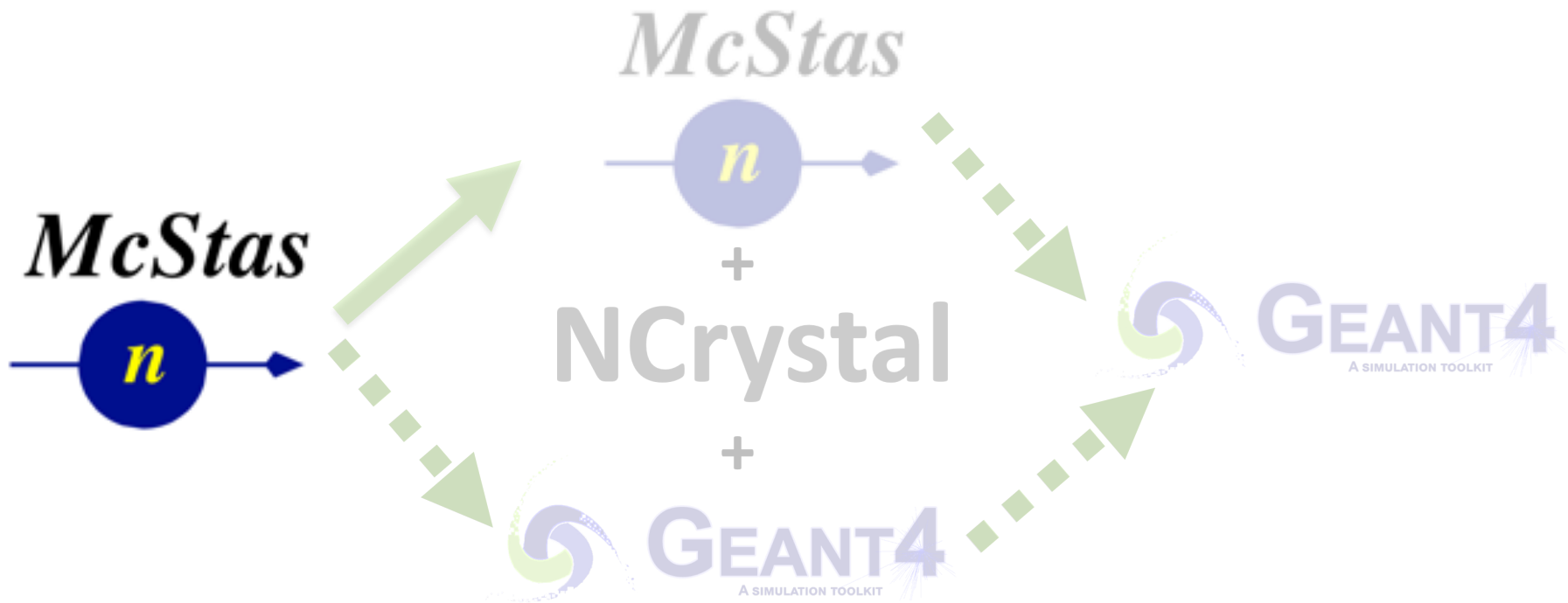
- Enables Monte Carlo simulation of neutrons in crystals
- Single-crystals
- Polycrystalline/powder materials
- **Anisotropic layered crystals: pyrolytic graphite**
- Coherent elastic (Bragg) diffraction
- Includes “background” (inelastic/incoherent)
 - Harmonic approximation
 - Incoherent approximation
 - Debye approximation

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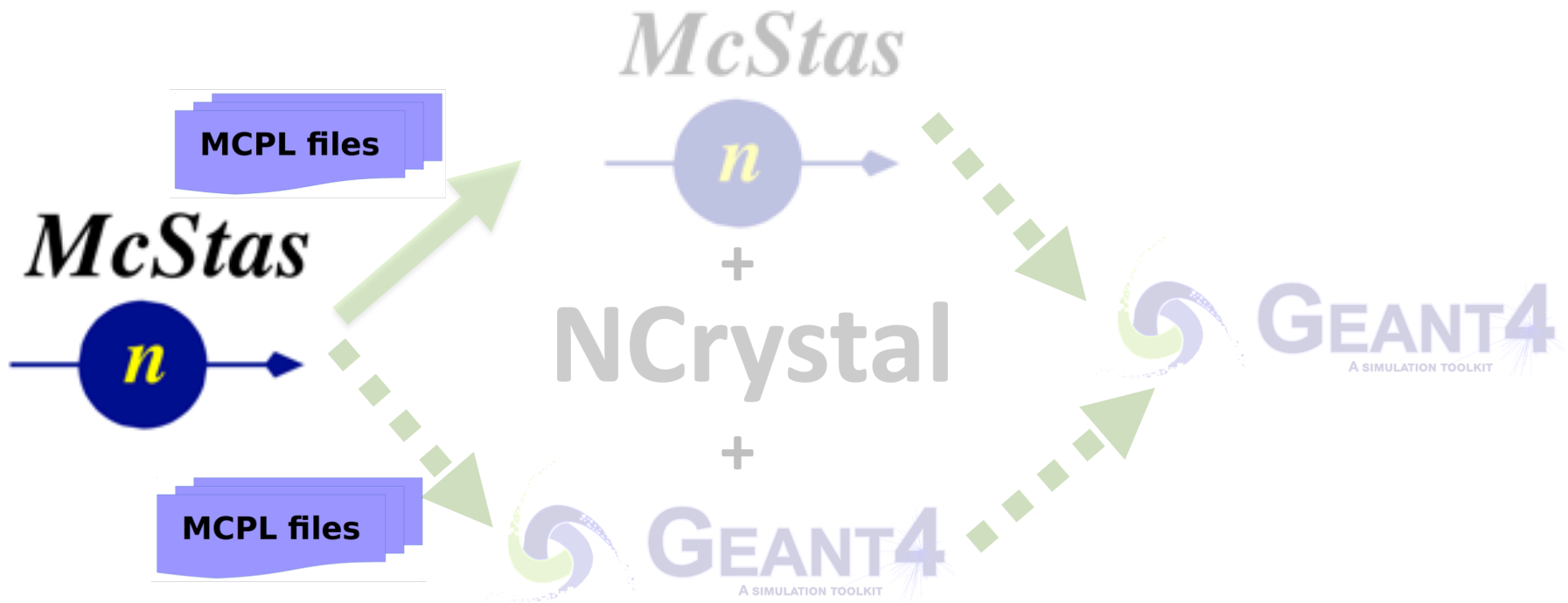


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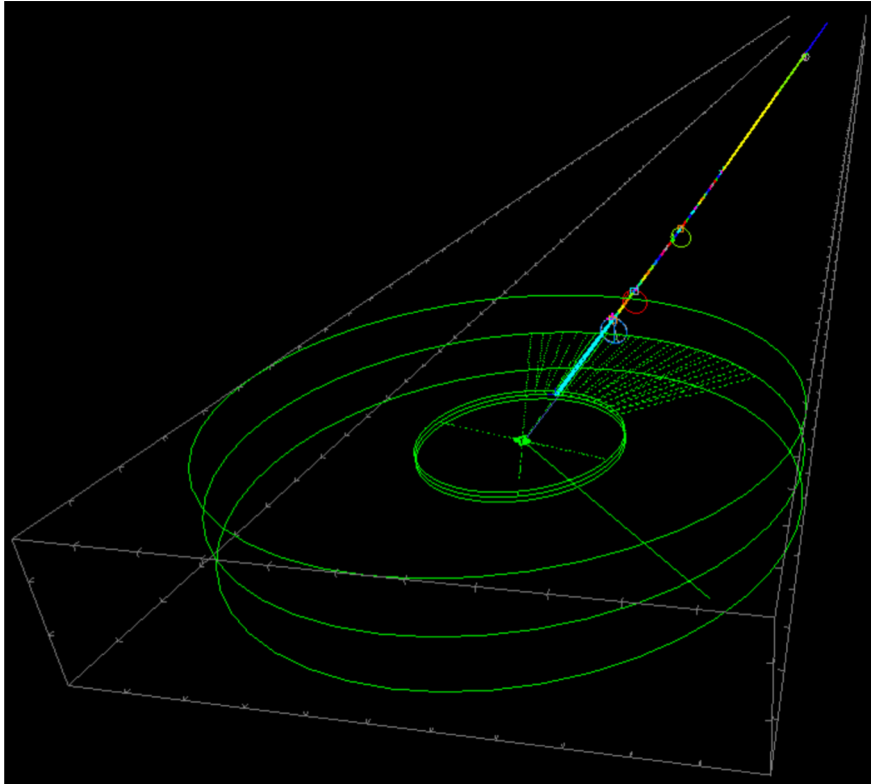
Detectors



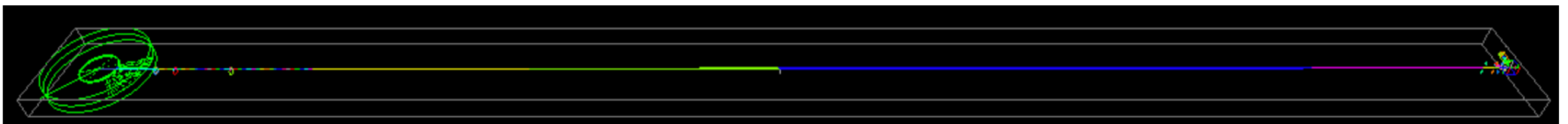
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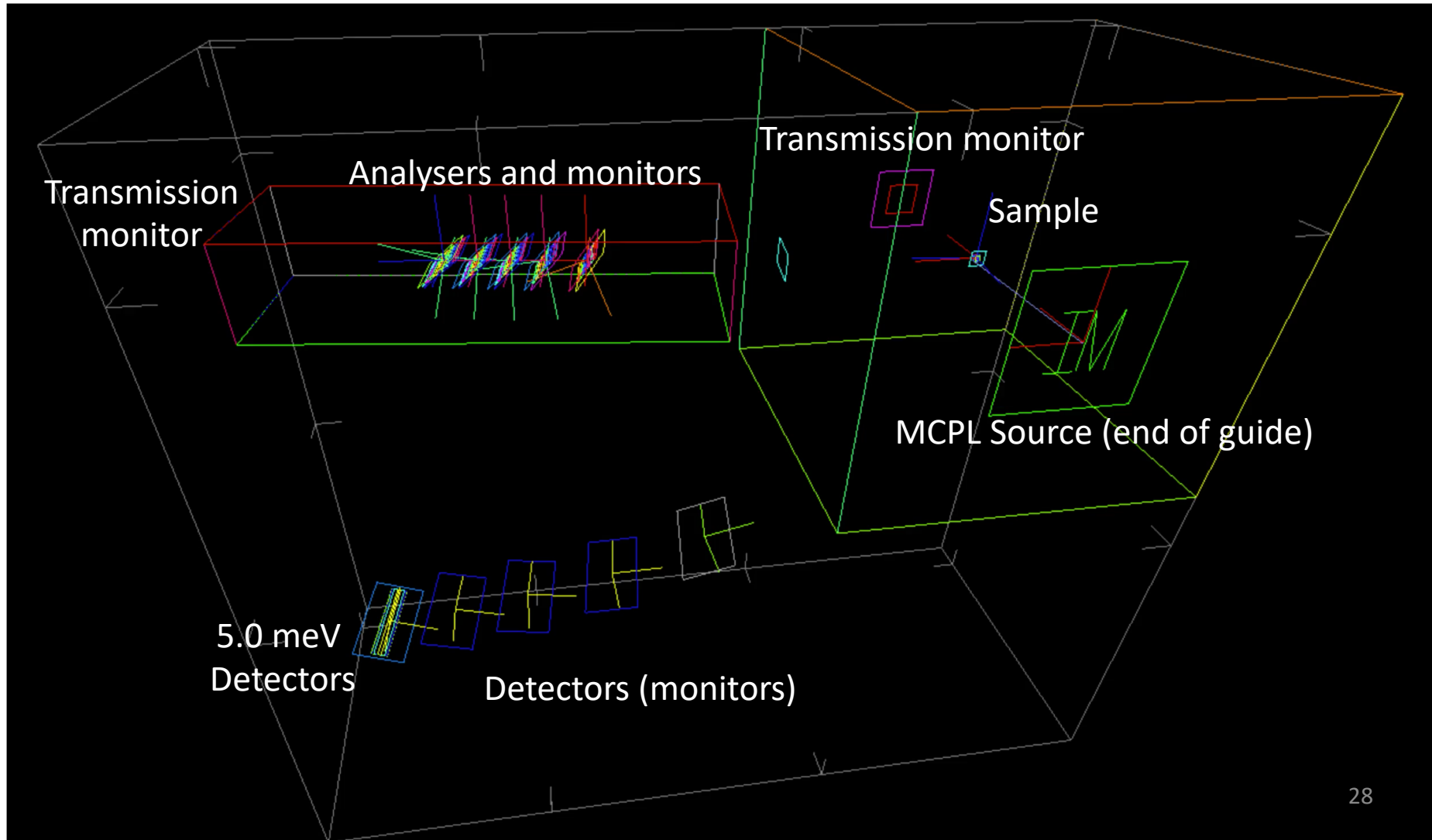
McStas Model – Full Instrument



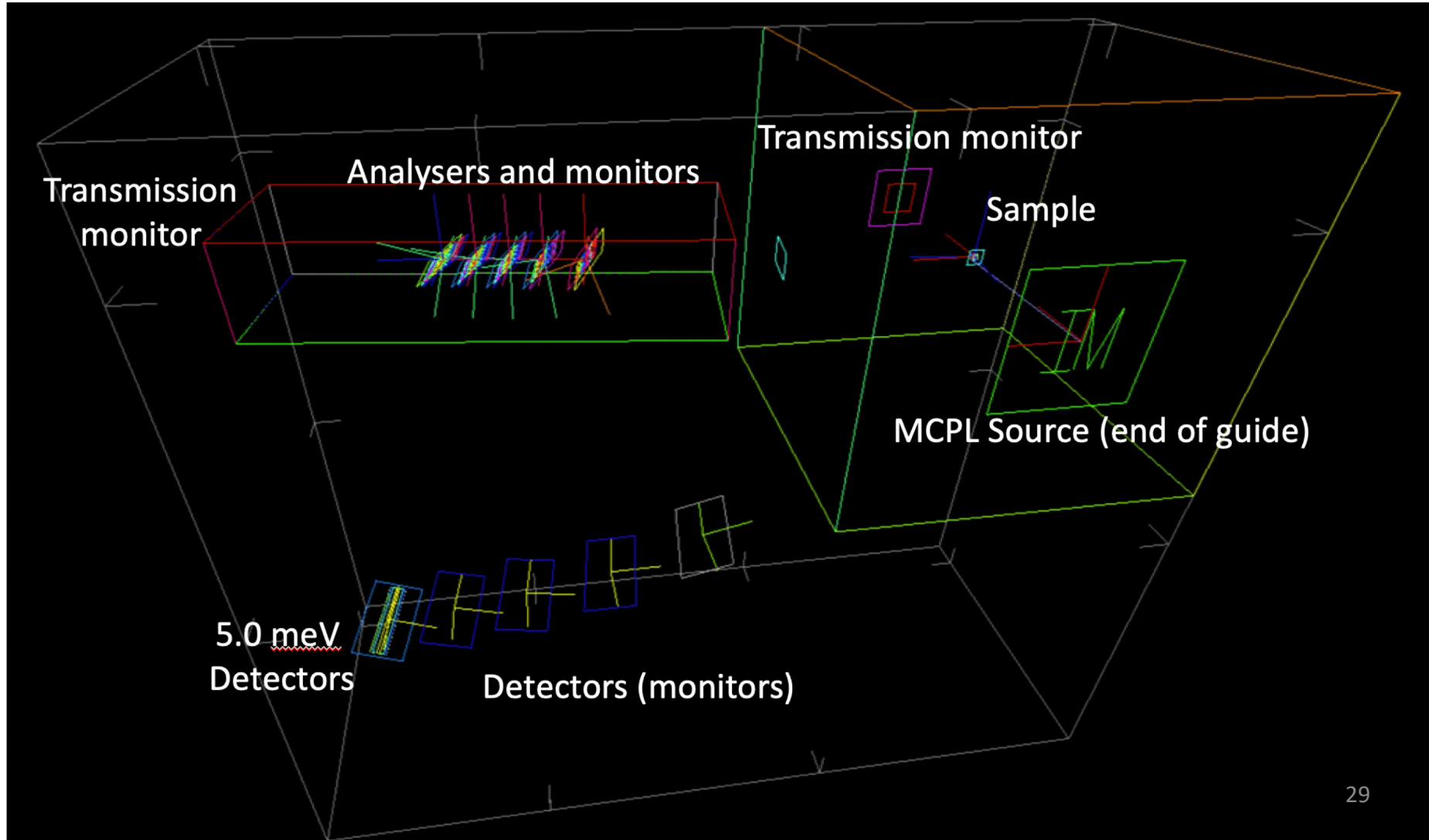
- ESS Butterfly source
- 4 choppers, all guide sections
- Authors:
Rasmus Toft-Petersen
Jonas Okkels Birk
Martin Olsen



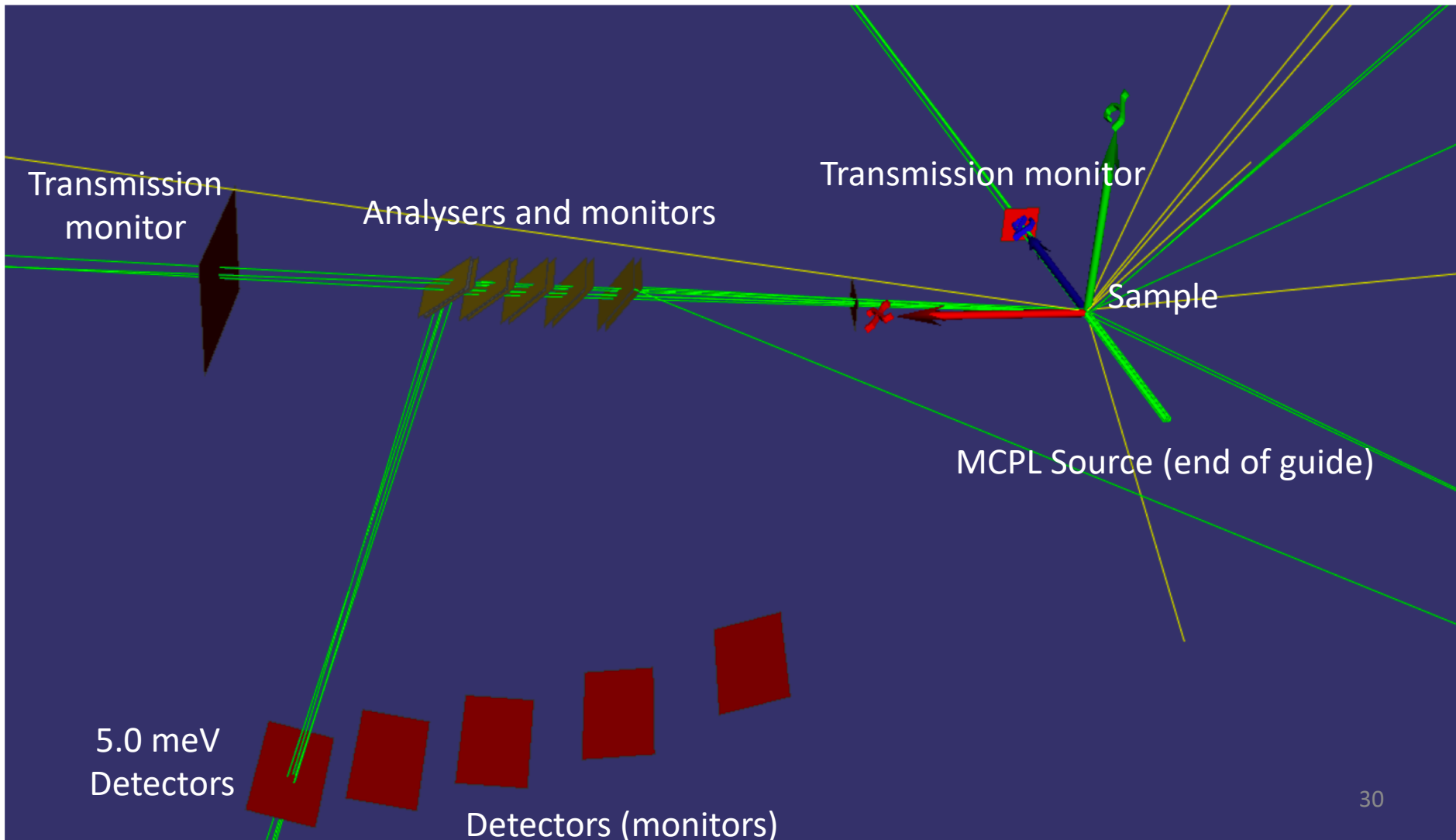
McStas Model – Analyzer-Detector system



McStas Model – Analyzer-Detector system



Geant4 Model – Analyzer-Detector system

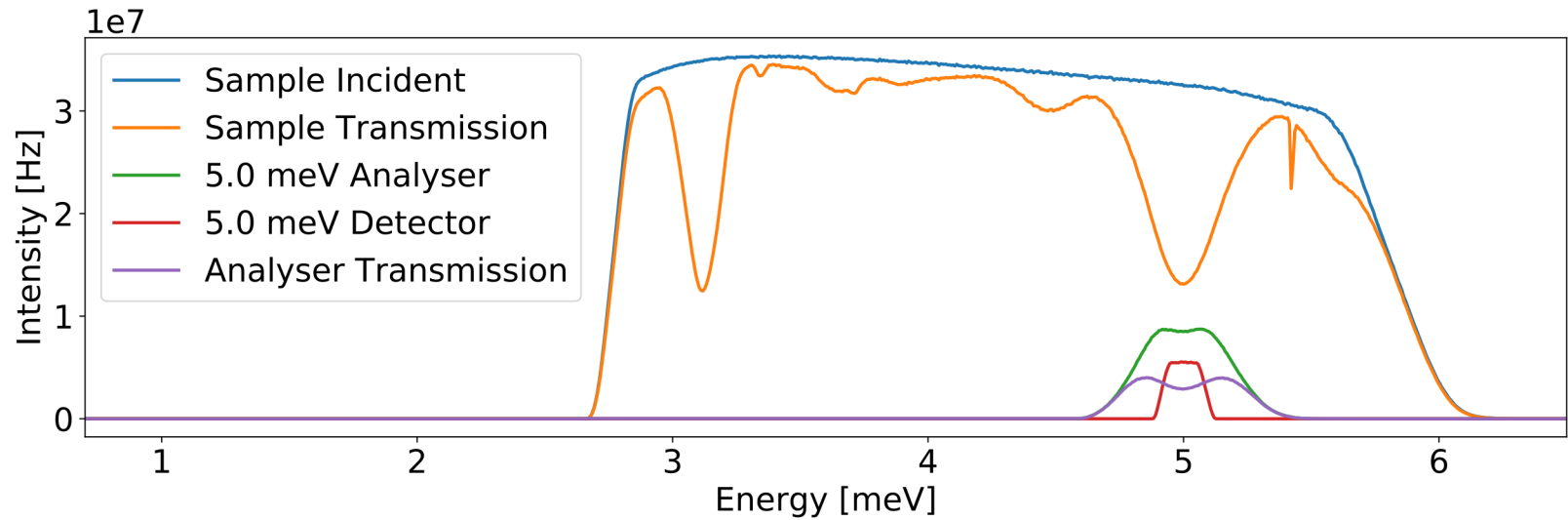


Outline

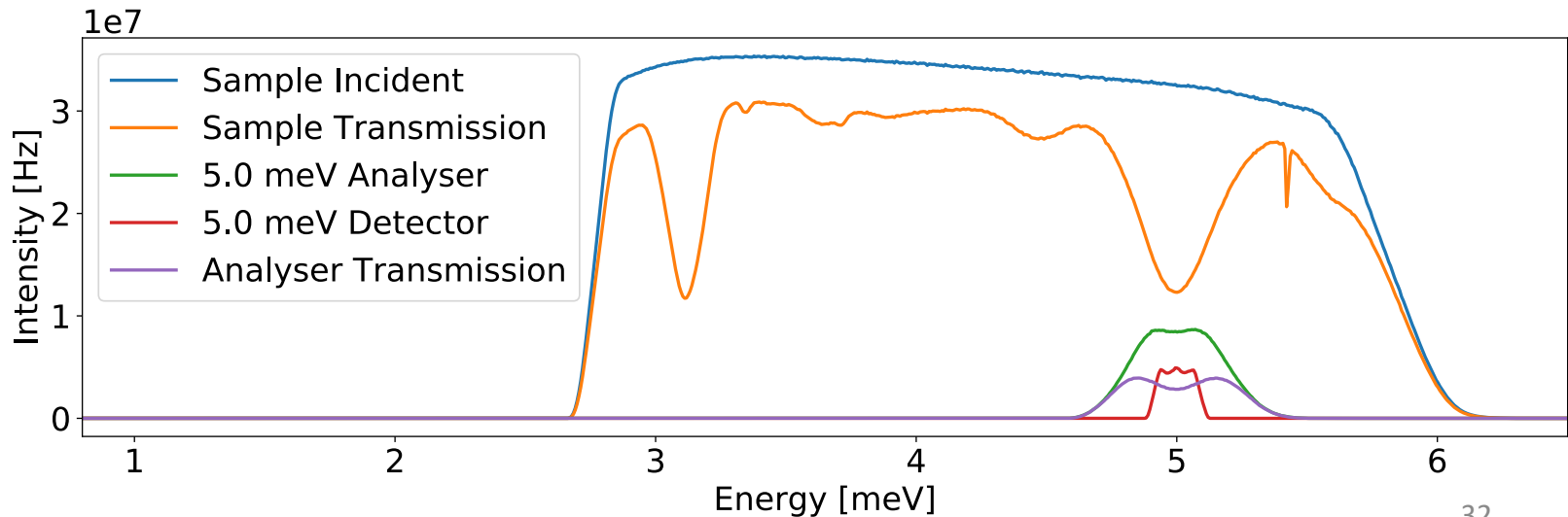
- BIFROST Instrument
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Change of energy spectrum after sample

McStas

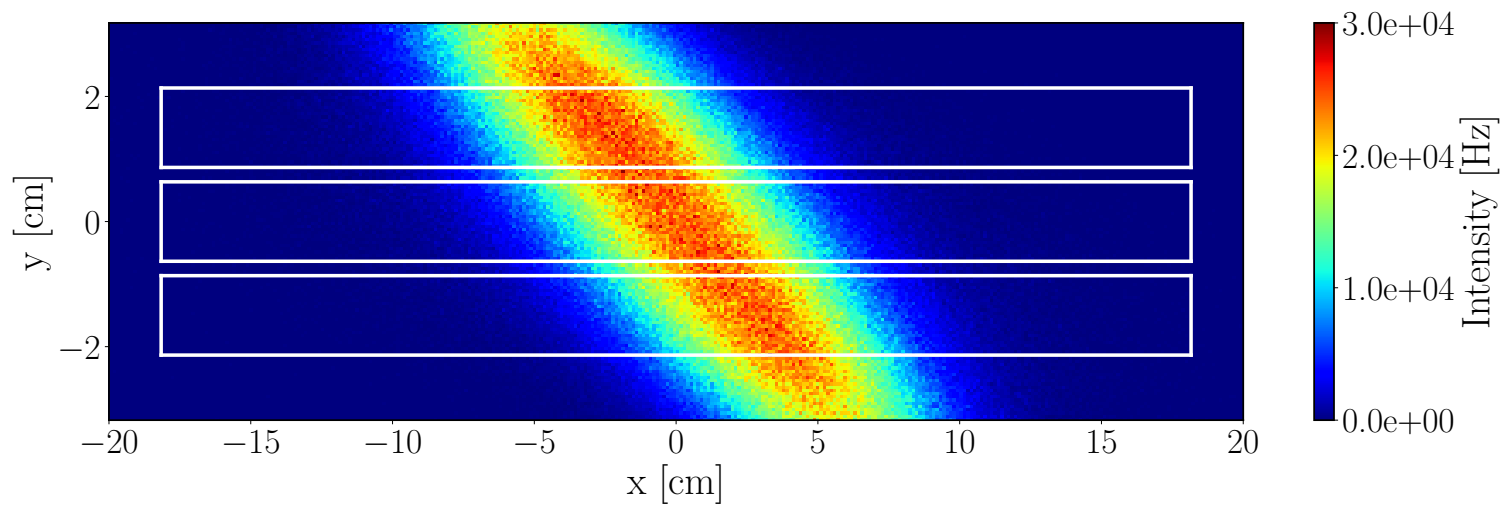


Geant4

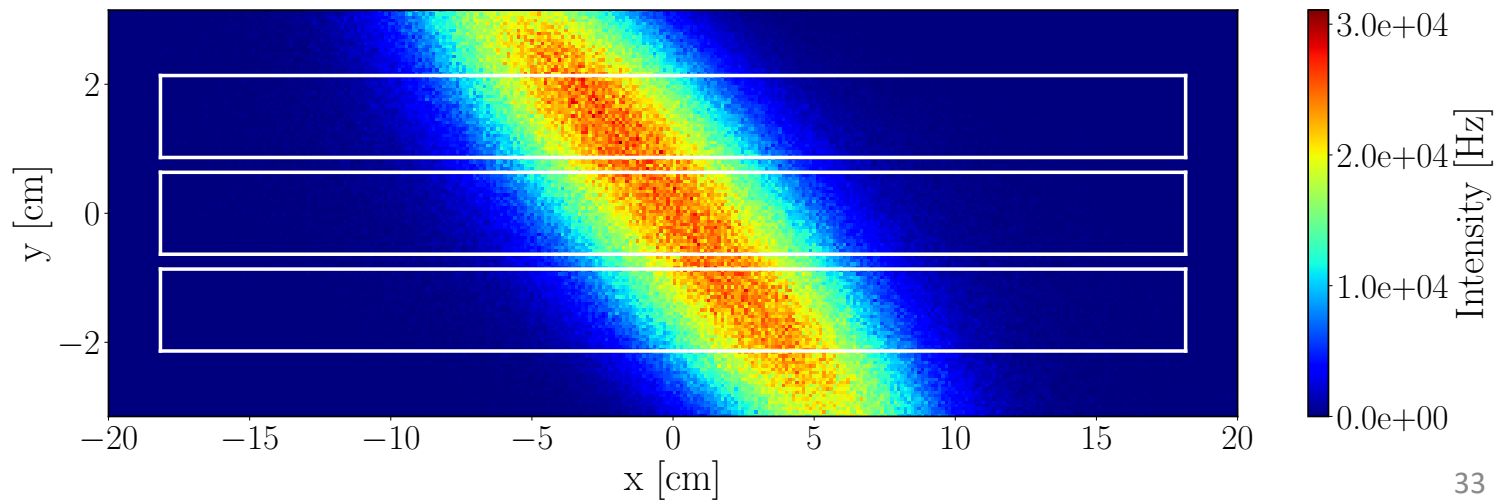


Intensity on detector

McStas

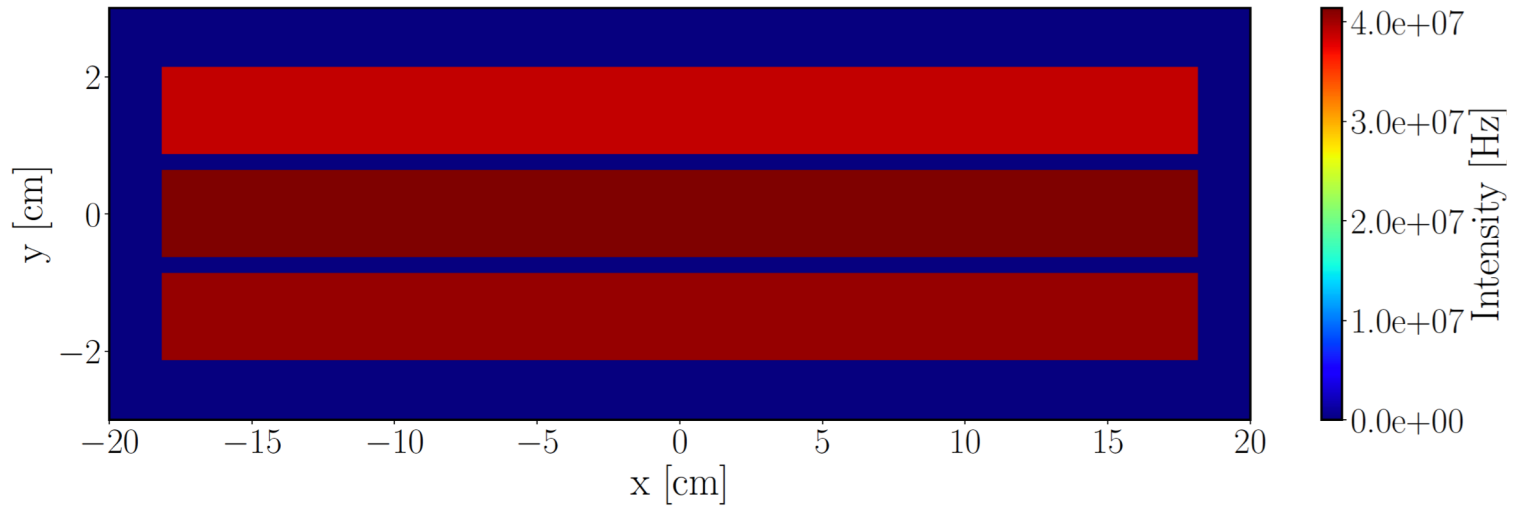


Geant4

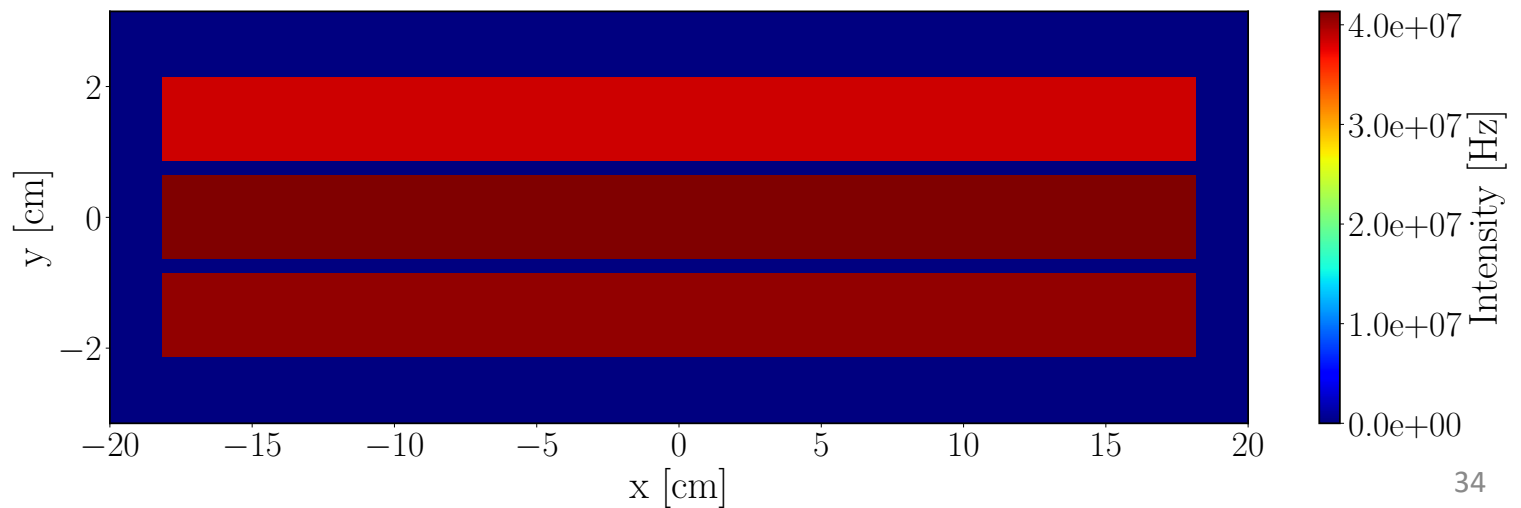


Time averaged incident rate

McStas

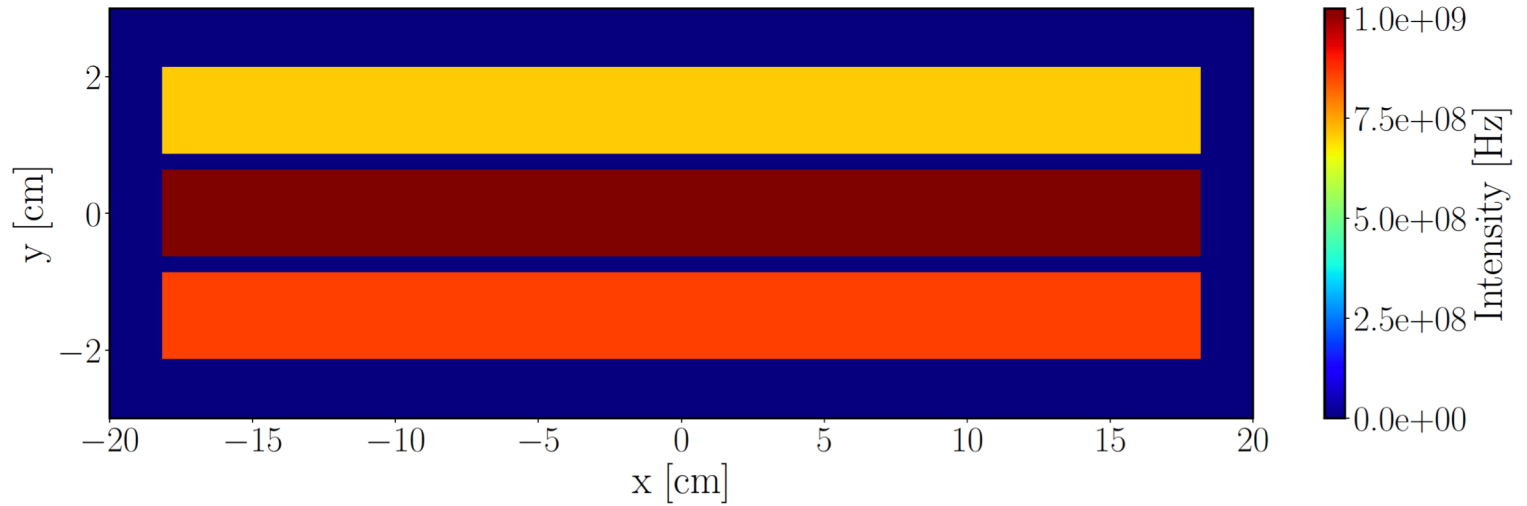


Geant4

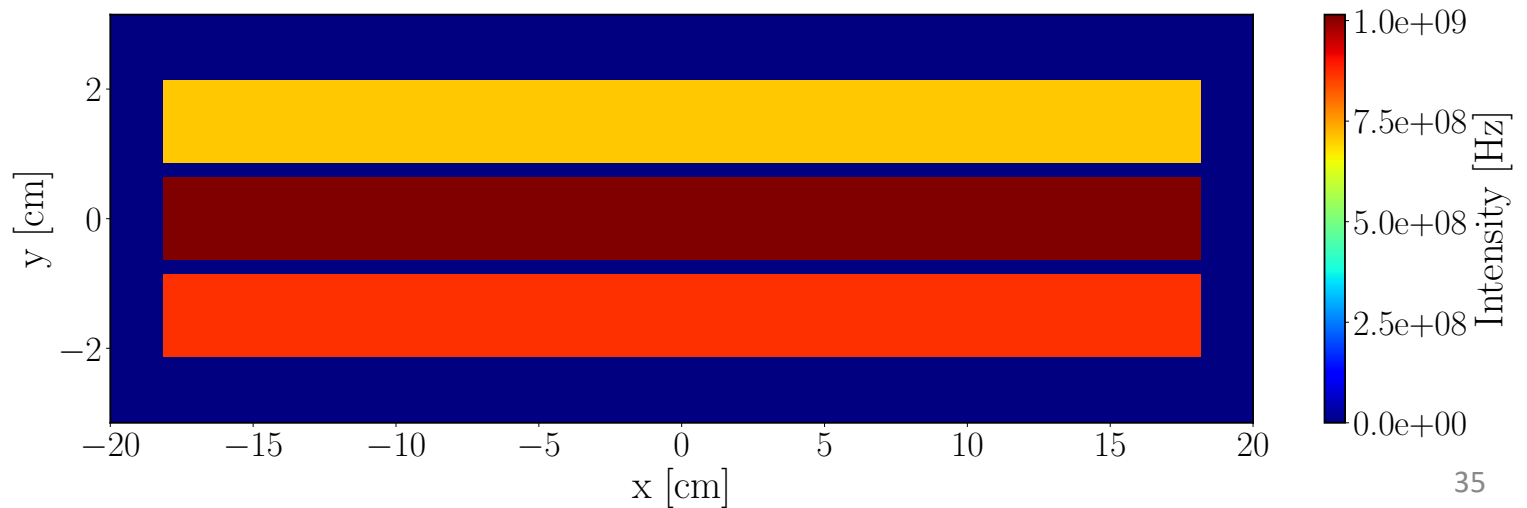


Peak instantaneous incident rate

McStas



Geant4

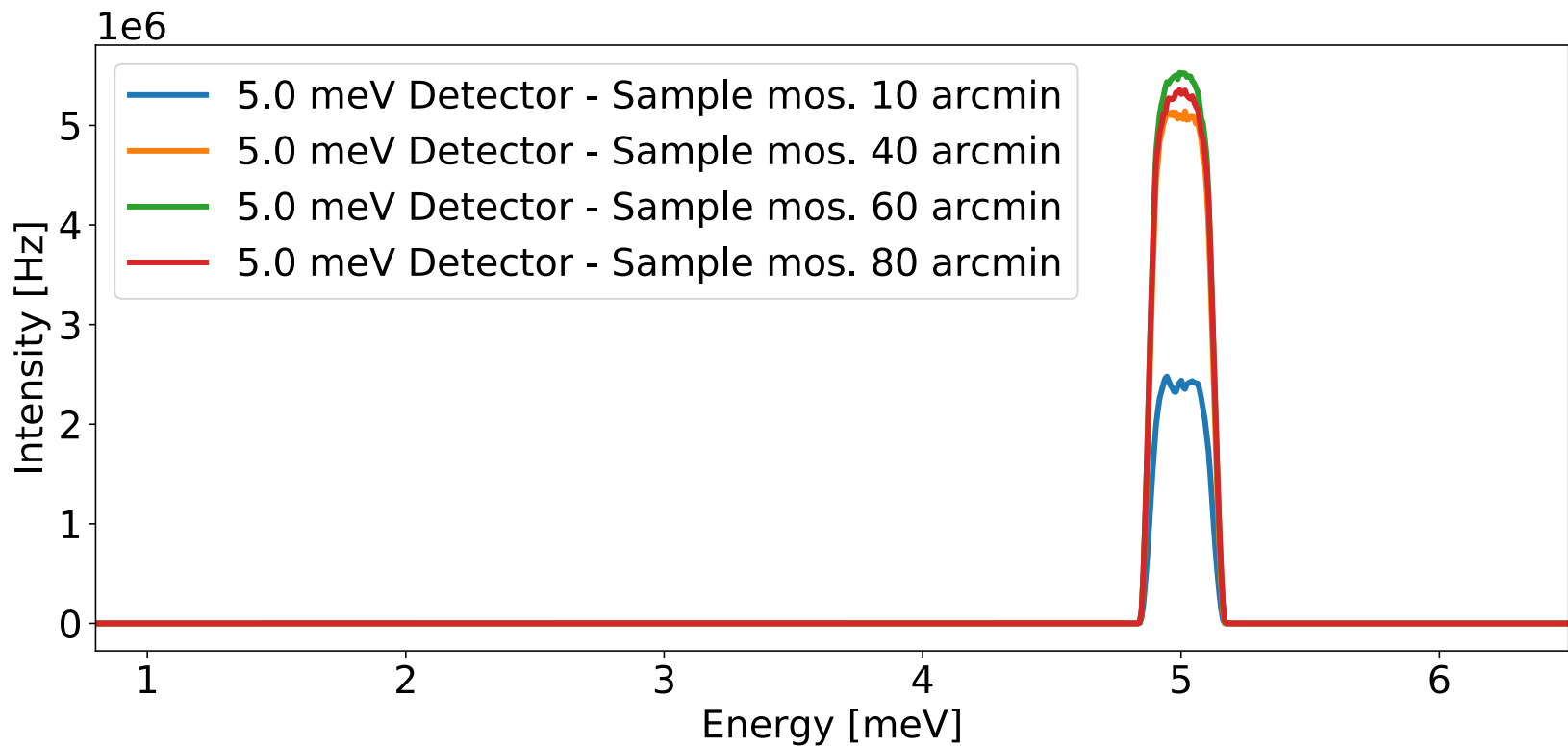


Conclusion

- Parameters:
 - Sample: Y_2O_3 single-crystal, $hkl=2,-2,-2$ ($d_{hkl} = 3.0724 \text{ \AA}$)
cylindrical $h=d=15 \text{ mm}$, mosaicity = 60 arcmin
 - Analyzer: thickness = 1 mm, mosaicity = 60 arcmin
 - Source power = 5 MW
 - PSC opening time = 5 ms (full ESS pulse)
- Time averaged incident rate on one He-3 tube: $4e7 \text{ Hz}$
- **Peak instantaneous incident rate on one tube: $1e9 \text{ Hz}$**

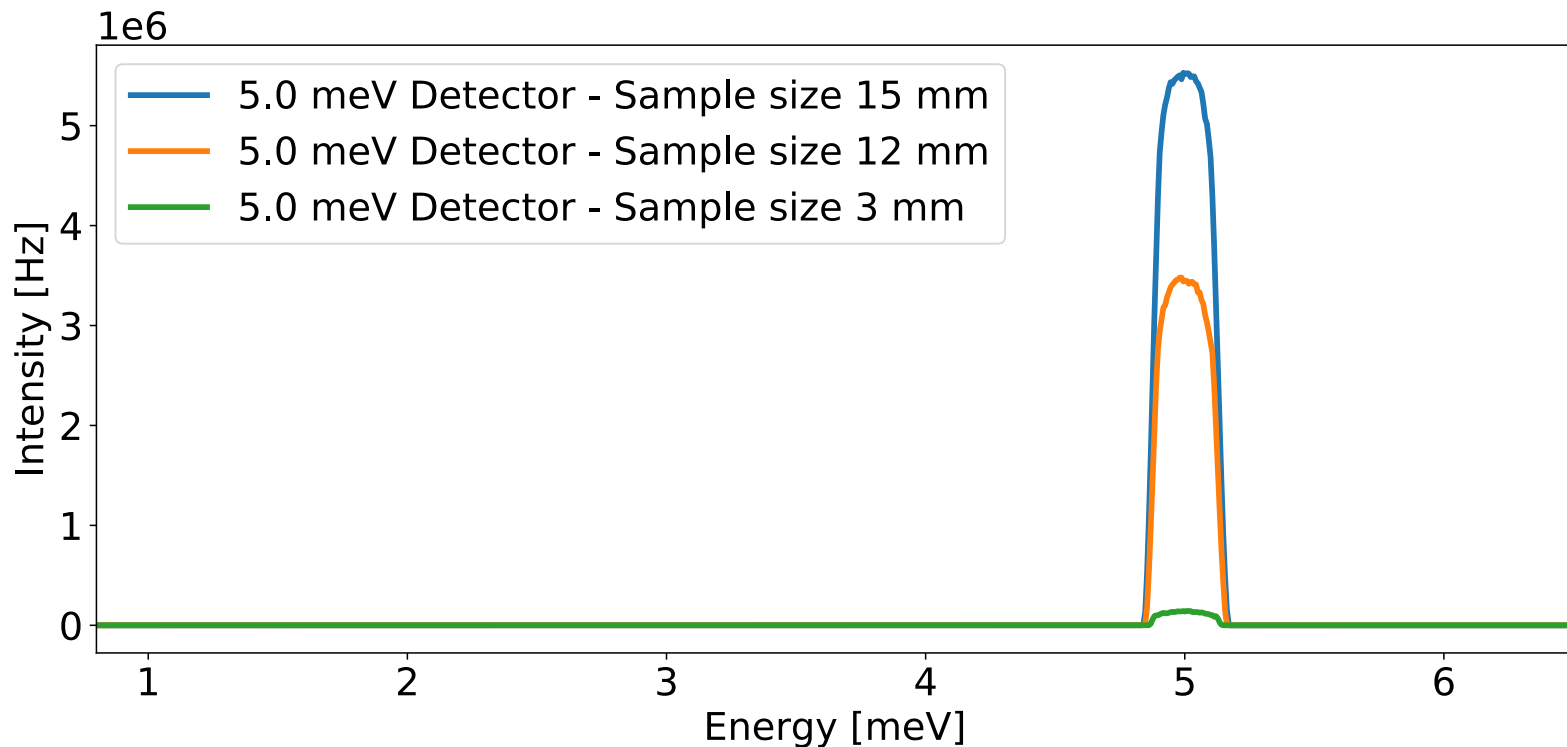
Effect of sample mosaicity

- Sample mosaicity matching the analyser mosaicity (60 arcmin) gives the highest incident rates



Effect of sample size

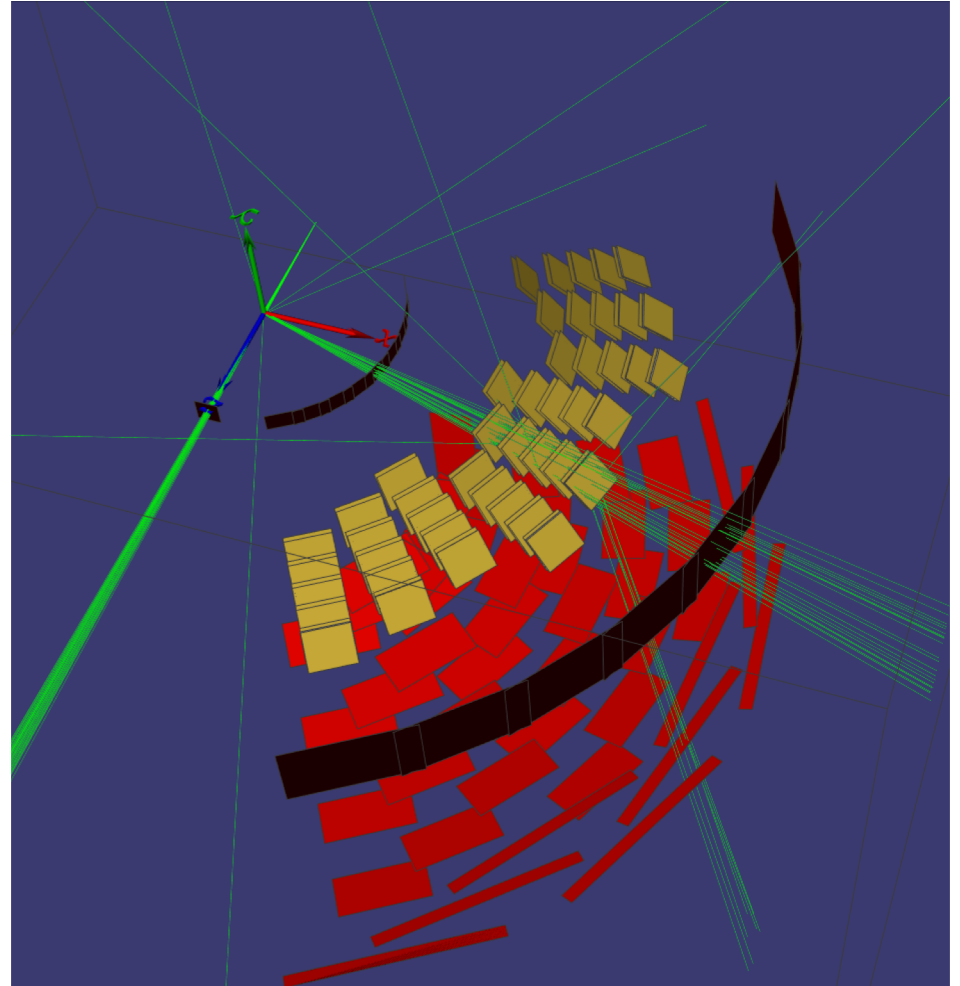
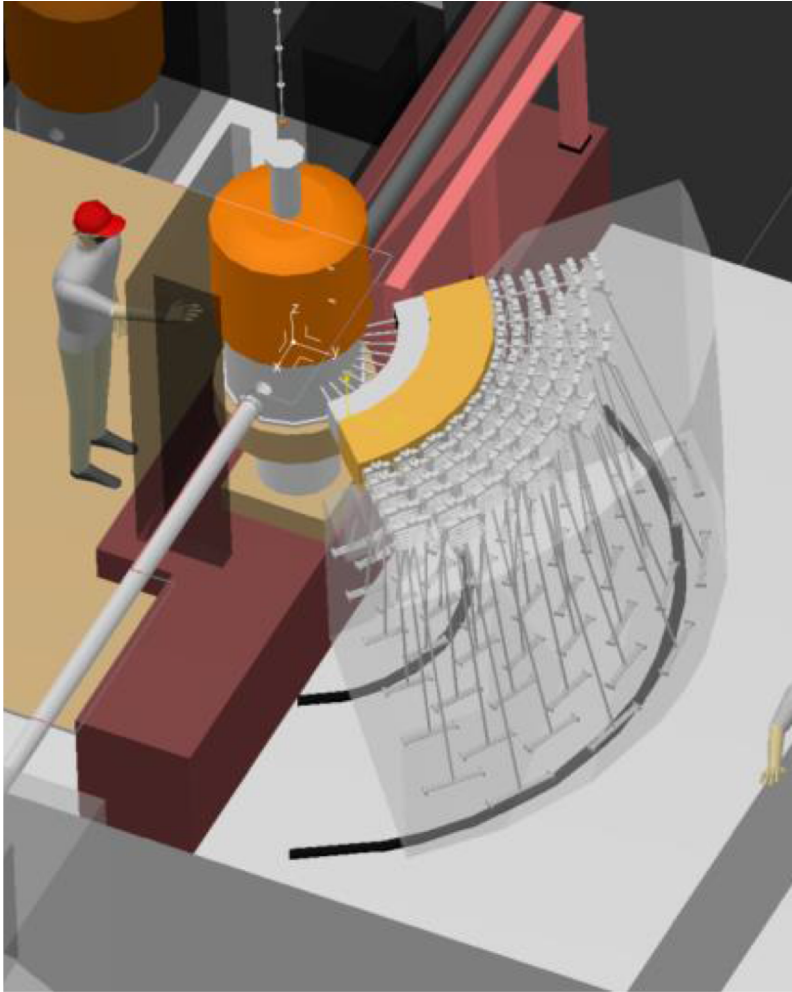
- Detector rates drop significantly with smaller sample size:
- 15 mm \rightarrow 12 mm ($h=d$) a factor of 1.4 rate drop
- 15 mm \rightarrow 3 mm ($h=d$) a factor of 40 rate drop



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Geant4 model with all Q channels



Ongoing and possible studies

- Simulation of calibration sample (vanadium) with full model
- Study the effect of PSC opening time on energy resolution and rates
- Beryllium filter + radial collimator
- Detectors
- Cross-talk shielding
- Backscattering
- Connect to Mantid

Acknowledgments

- Xiao Xiao Cai, Peter Willendrup
- Data Management&Software Centre (DMSC)

Thank you for your
attention!