



I have only worked on McStas related
projects and it has been great

Mads Bertelsen

McStas 25th Anniversary, 1998 - 2023

McStas simulations as a career?



“Simulations and software is a good skill to have,
but you must find a main science topic to be employed.”

I think there is space for support scientists

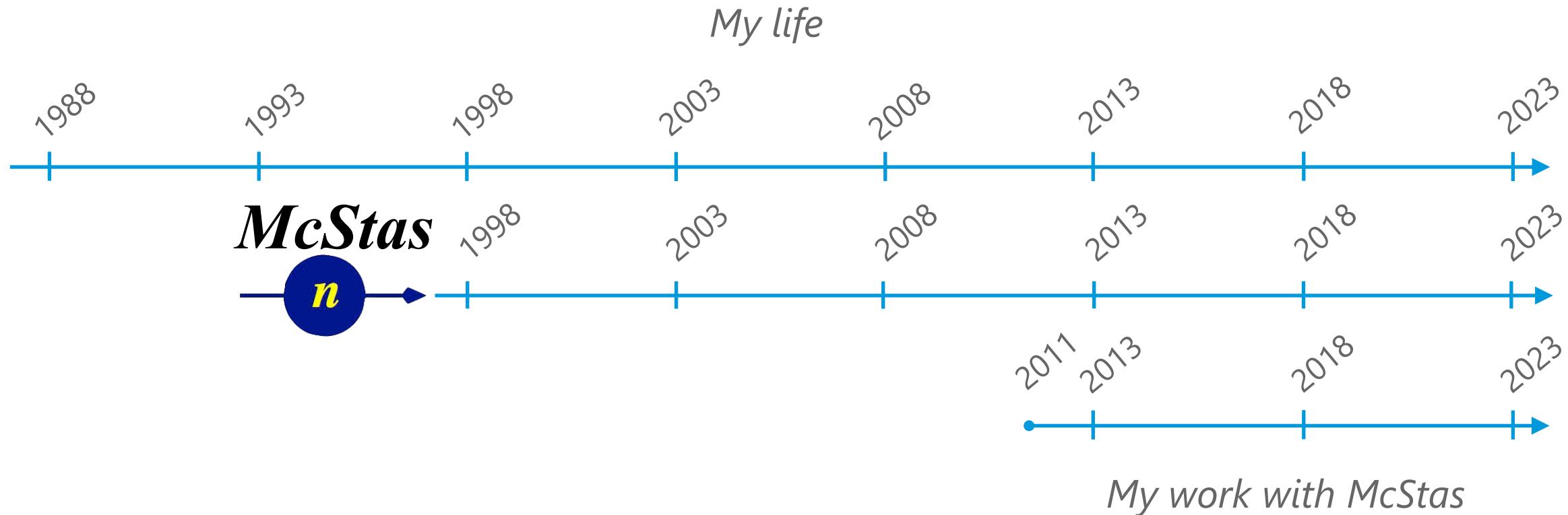
Timeline

Overview



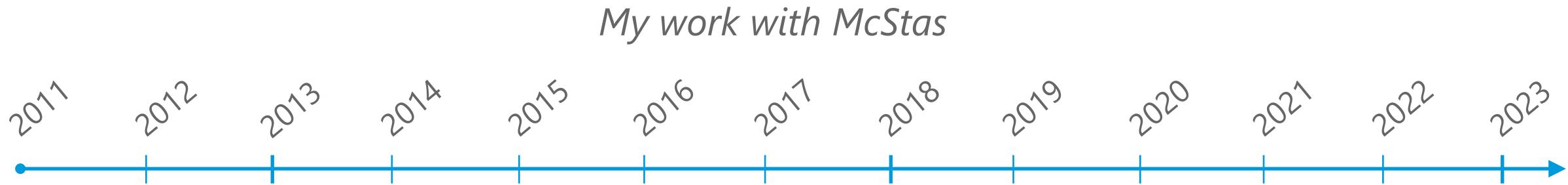
Timeline

Overview



Timeline

Overview



Timeline Overview

University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



Position



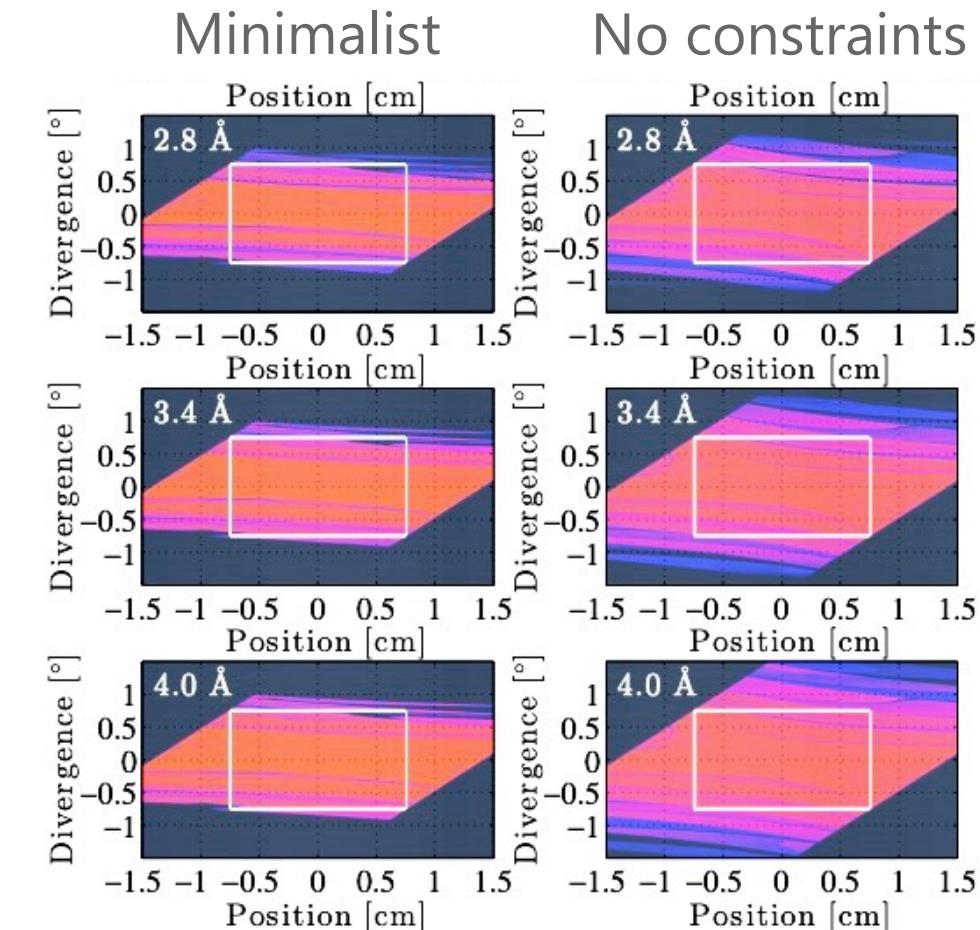
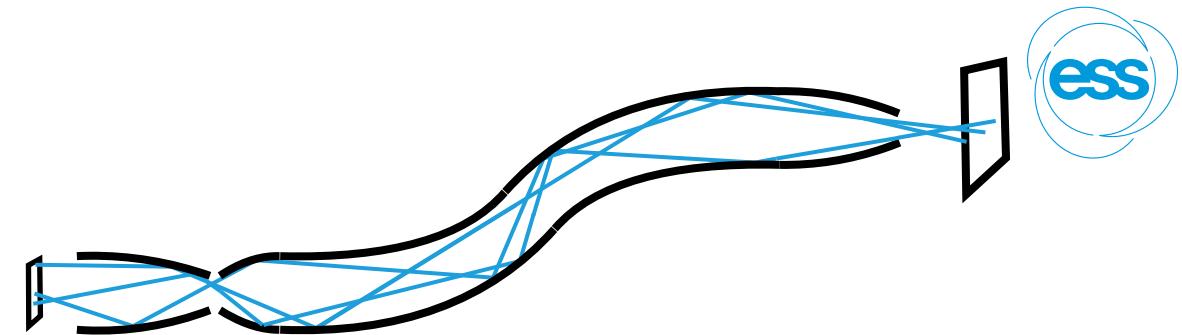
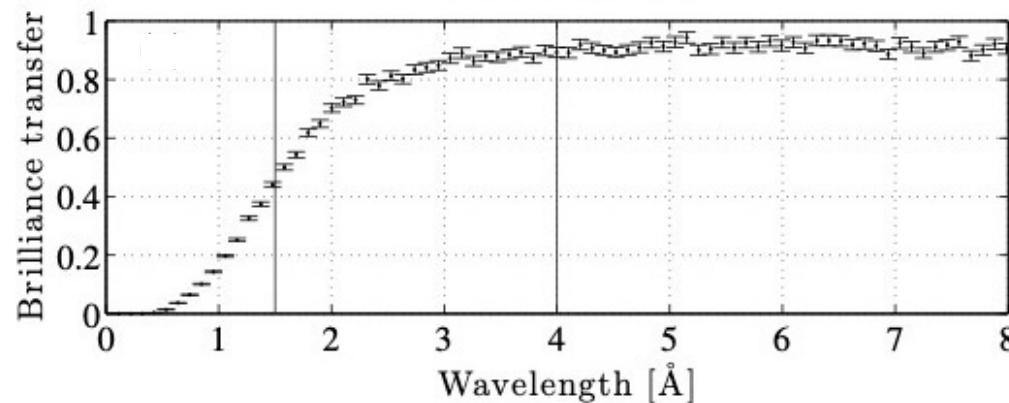
Subject



Guide design

A repetitive task

- Iterations of beam requirements
- Frequent rule changes from ESS
- Optimization for brilliance transfer with MATLAB + iFit
- Minimalist principle



Timeline Overview

University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



Position



Subject



Software

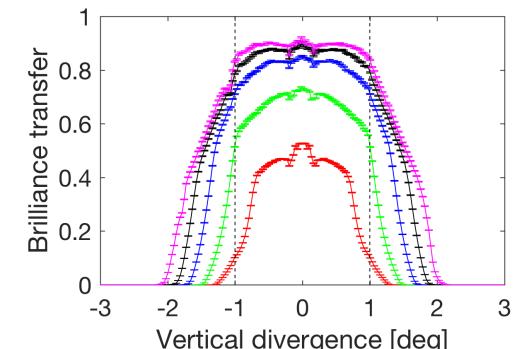
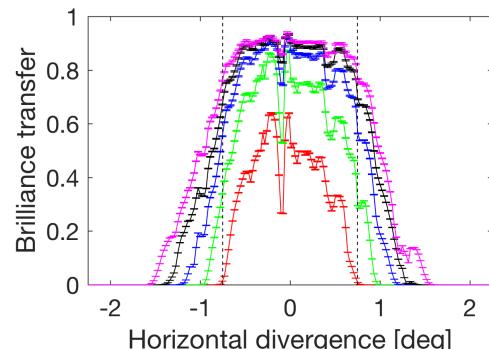
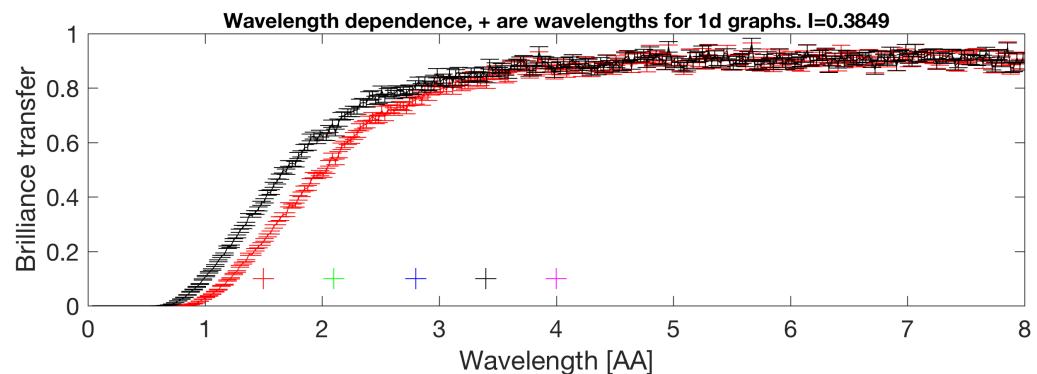
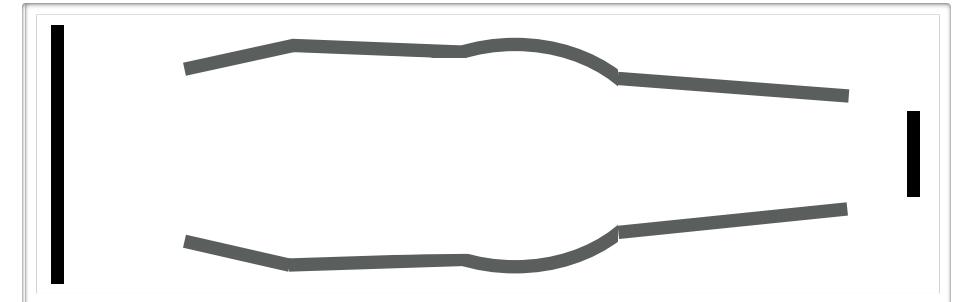


guide_bot

MATLAB Version

- Optimization of neutron guides
- Simple input for
 - Beam requirements
 - Source
 - Guide geometry
- Automated steps
 - Builds McStas simulations
 - Performs numerical optimization (iFit)
 - Characterizes the optimal guide

S S S



guide_bot

MATLAB Version

- Optimization of neutron guides
- Simple input for
 - Beam requirements
 - Source
 - Guide geometry
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 - Builds McStas simulations
 - Performs numerical optimization (iFit)
 - Characterizes the optimal guide
- ESS
 - BIFROST
 - HEIMDAL
 - MIRACLES
 - VESPA
 - ESPRESSO
- PSI
 - CAMEA
 - FOCUS



Timeline Overview

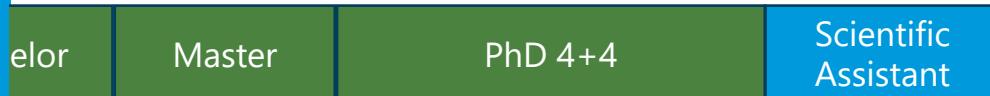
University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



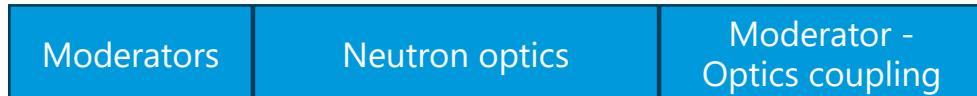
Position



Job description

"Investigate pancakes and doughnuts."

Subject



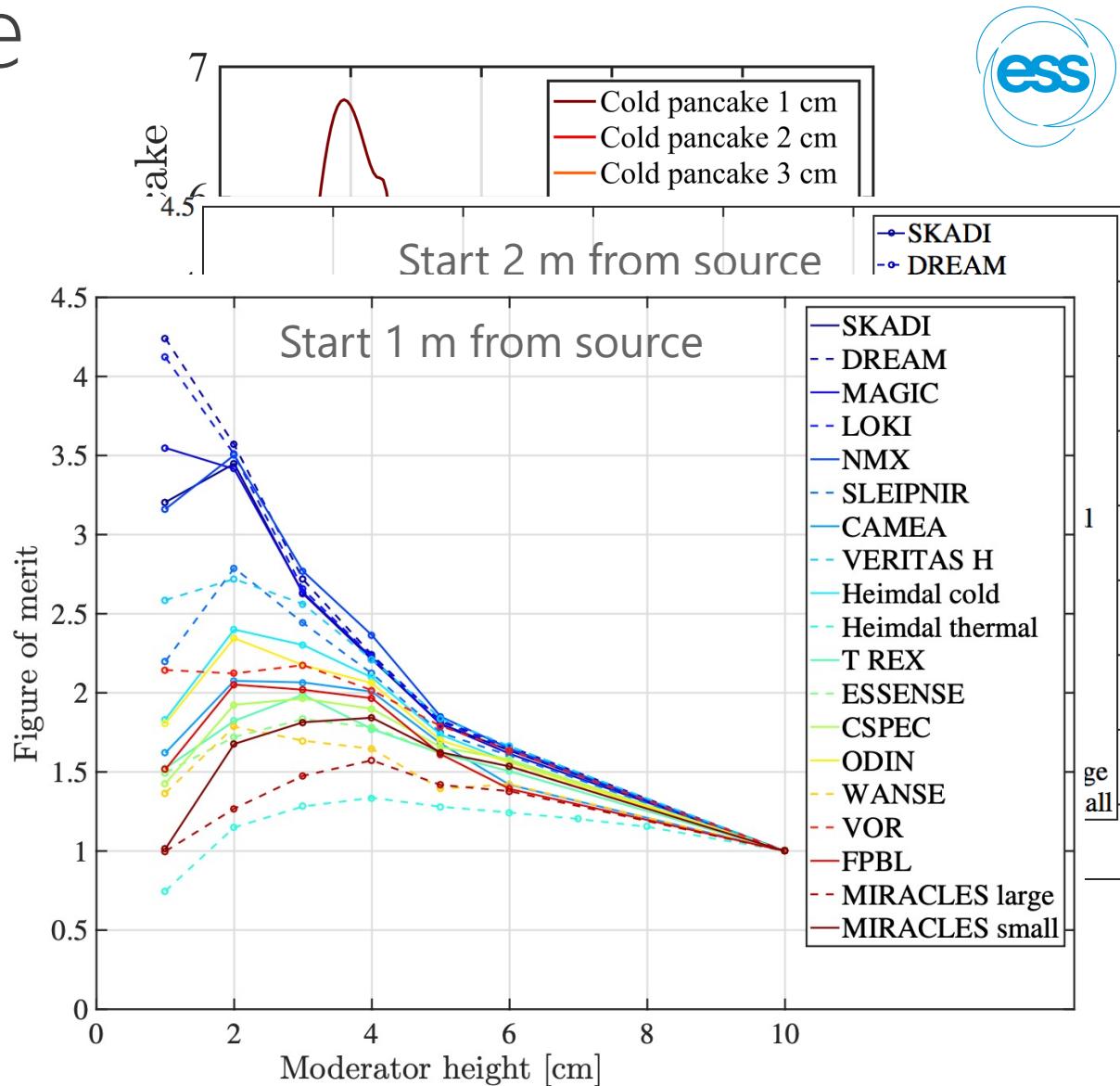
Software



ESS moderator choice

MATLAB Version

- Reoptimize guides for ESS instruments under consideration
- Collaborated with almost all instrument teams
- Some performed their own optimizations
- Optimized more than 15000 guides
- Approximately 15 million McStas runs
- A 3 cm tall moderator was chosen



Timeline Overview

University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



Position



Subject

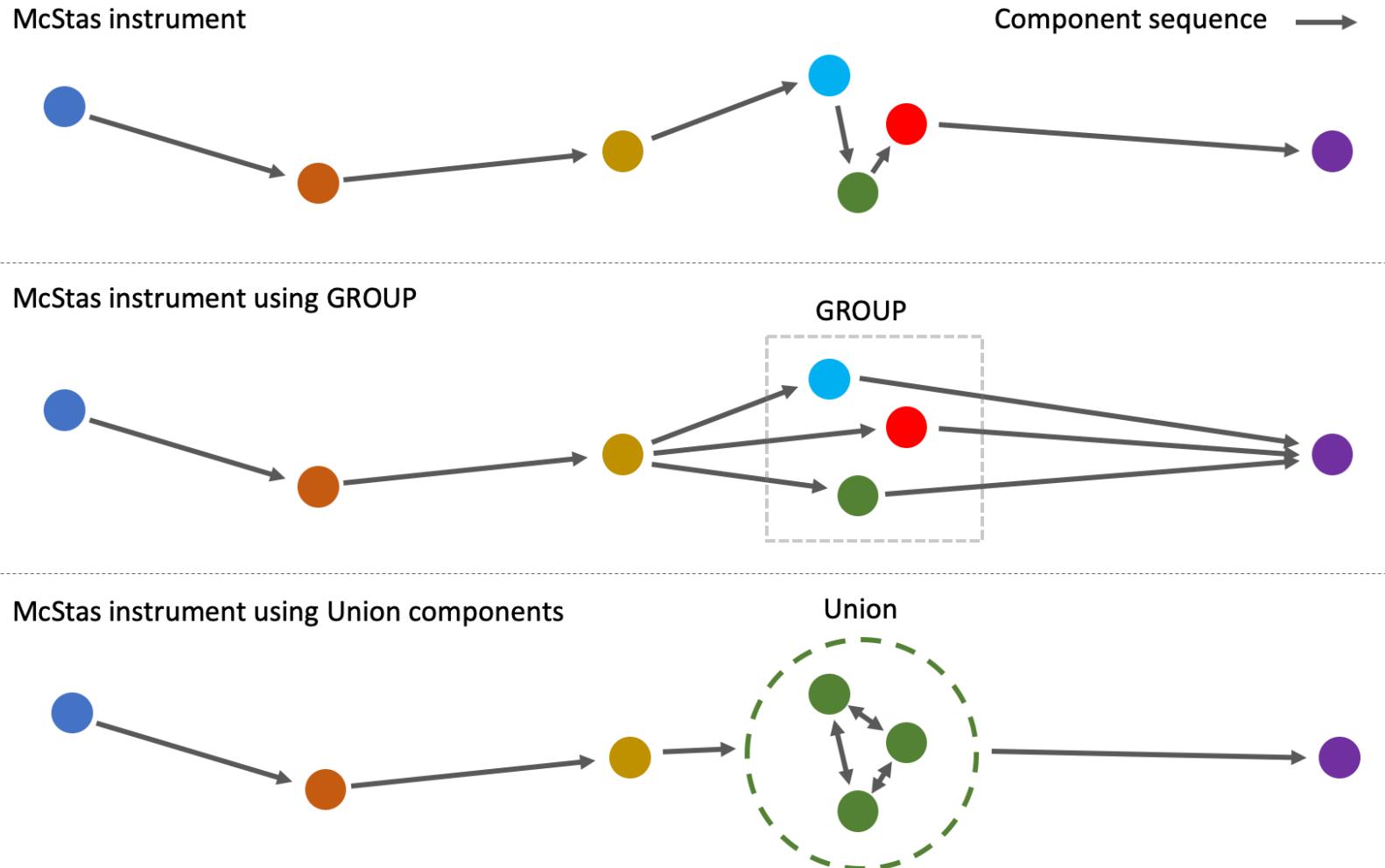


Software



Union components

Union in the instrument

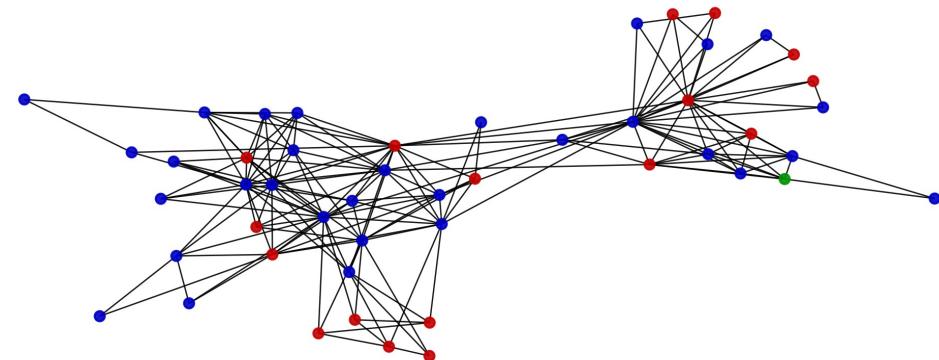
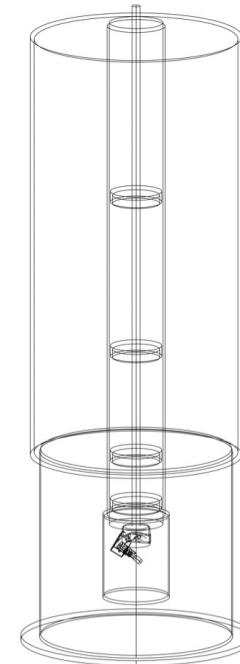
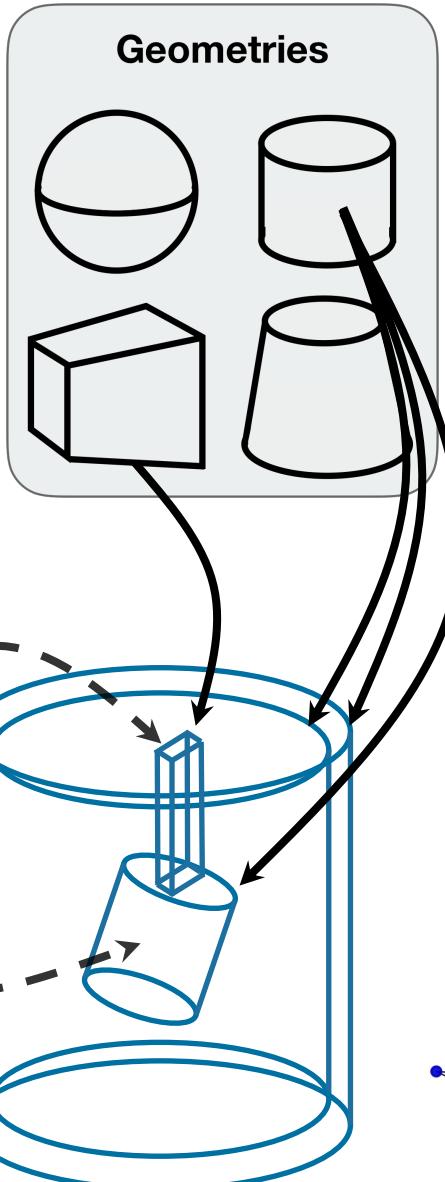
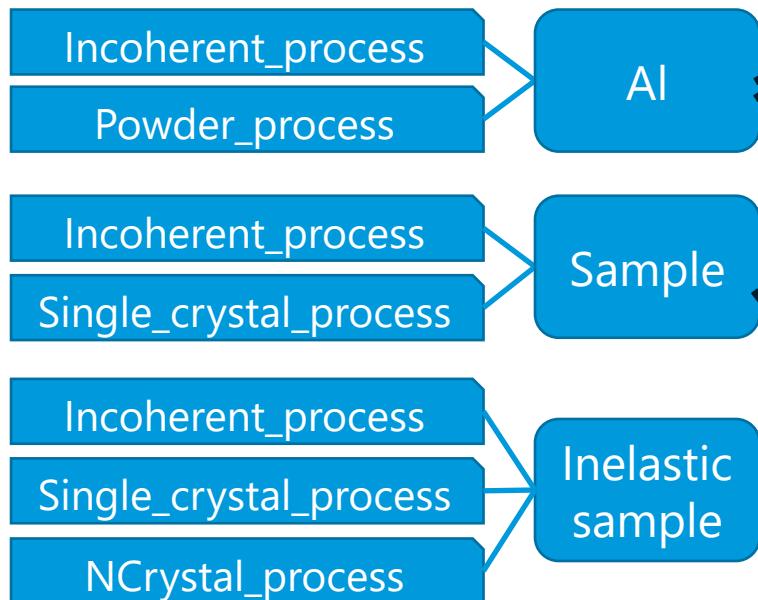


Union components

Overview

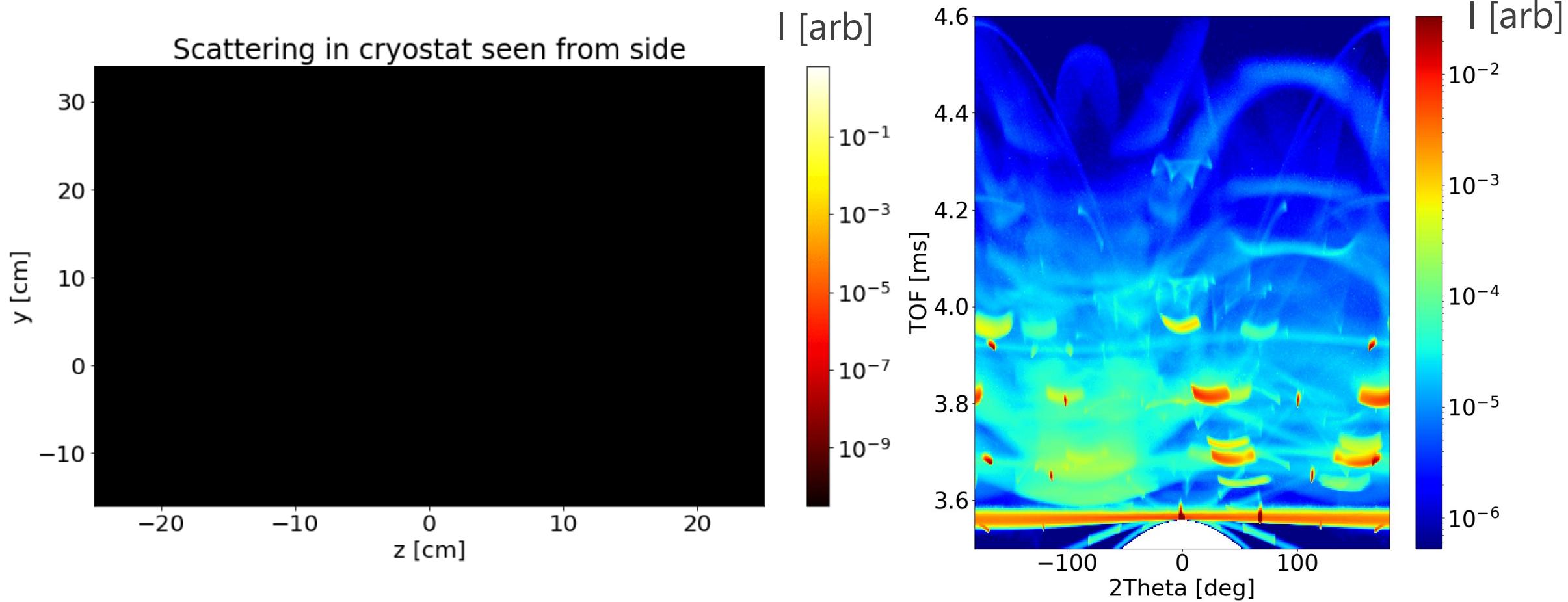
- Set of McStas components
- Works as a collection

Physics



Union components

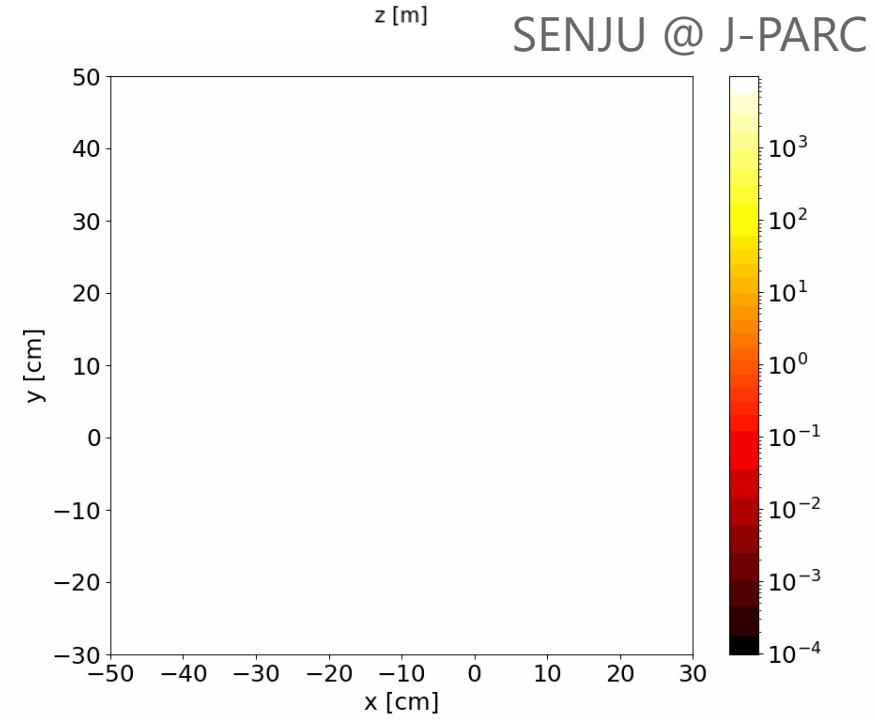
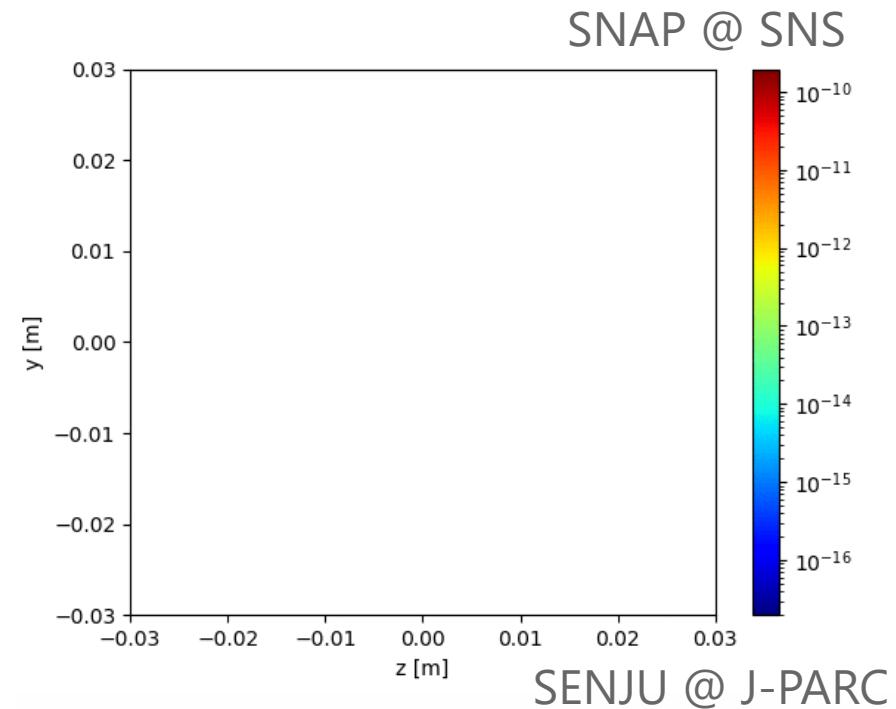
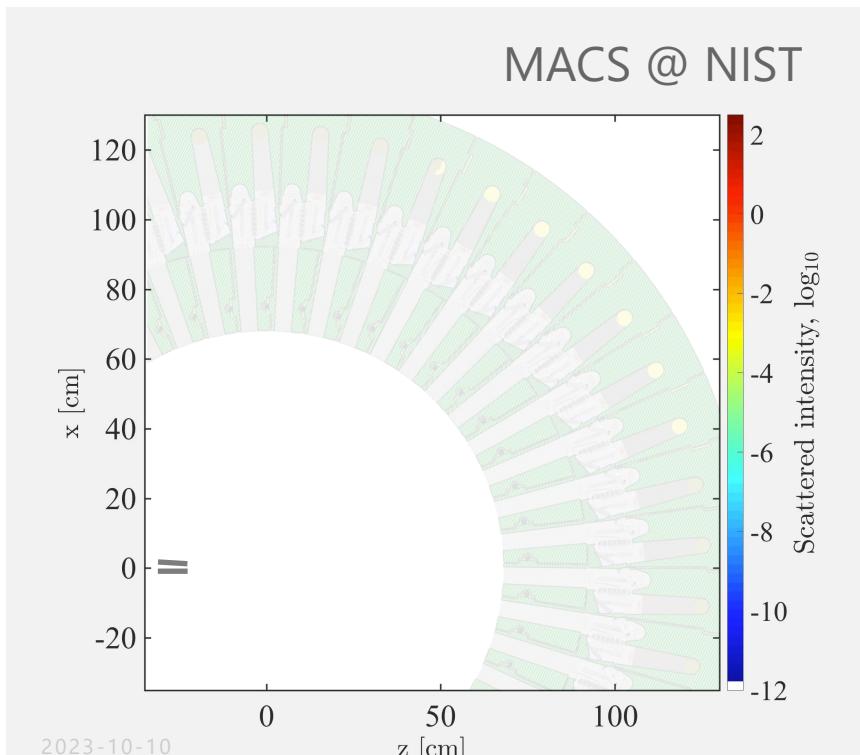
Results



Union components

Instruments

- Joined beamtimes
- Simulated the instruments



Timeline Overview

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European Spallation Source



My work with McStas



Position



Subject



Software

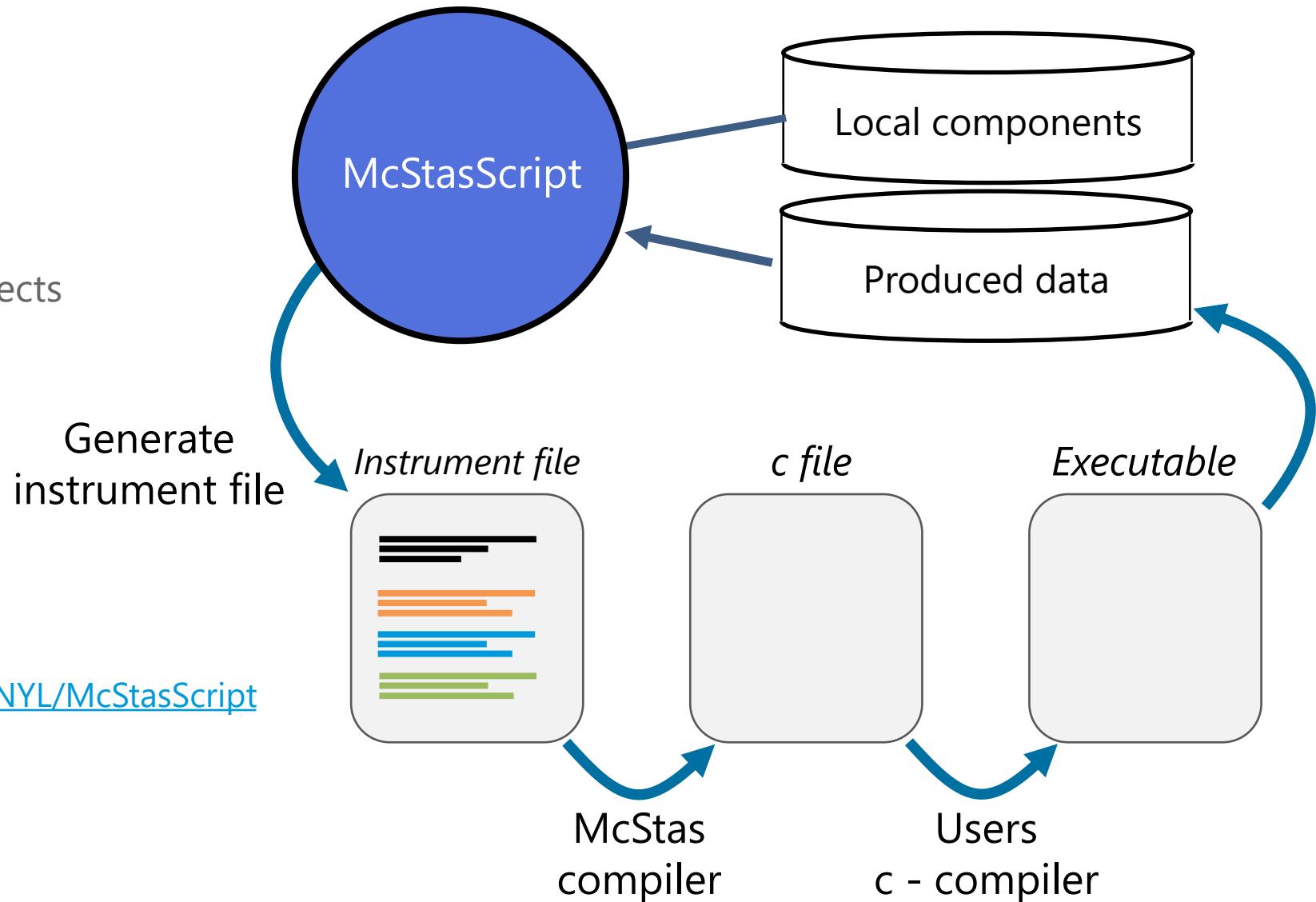


McStasScript

An alternate user interface

- Python McStas API
 - Build instrument object
 - Execute simulation
 - Receive data as Python objects

- Open source
- <https://github.com/PaNOSC-ViNYL/McStasScript>
- Comprehensive test suite



McStasScript

Quick demo

- Instrument object
- Knows components



```
import mcstasscript as ms

instrument = ms.McStas_instr("demo_instrument")

instrument.component_help("Source_div")
```

```
____ Help Source_div _____
|optional parameter|required parameter|default value|user specified value|
xwidth [m] // Width of source
yheight [m] // Height of source
focus_aw [deg] // FWHM (Gaussian) or maximal (uniform) horz. width divergence
focus_ah [deg] // FWHM (Gaussian) or maximal (uniform) vert. height divergence
E0 = 0.0 [meV] // Mean energy of neutrons.
dE = 0.0 [meV] // Energy half spread of neutrons.
lambda0 = 0.0 [Ang] // Mean wavelength of neutrons (only relevant for E0=0)
dlambda = 0.0 [Ang] // Wavelength half spread of neutrons.
gauss = 0.0 [0|1] // Criterion
flux = 1.0 [1/(s cm 2 st energy_unit)] // flux per energy unit, Angs or meV
```

McStasScript

Quick demo

- Component object
- Spots errors

- Autocompletion



```
src = instrument.add_component("source", "Source_div")
src.set_parameters(xwidth= 0.1, focus_aw=1.2, focus_ah=2.3,
                    lambda0=4.0, dlambda=0.1)

print(src)
```

```
COMPONENT source = Source_div(
    xwidth = 0.1, // [m]
    yheight : Required parameter not yet specified
    focus_aw = 1.2, // [deg]
    focus_ah = 2.3, // [deg]
    lambda0 = 4.0, // [Ang]
    dlambda = 0.1 // [Ang]
)
AT (0, 0, 0) ABSOLUTE
```

```
src.yheight= 0.05
print(src)
```

```
COMPONENT source = Source_div(
    xwidth = 0.1, // [m]
    yheight = 0.05, // [m]
    focus_aw = 1.2, // [deg]
    focus_ah = 2.3, // [deg]
    lambda0 = 4.0, // [Ang]
    dlambda = 0.1 // [Ang]
)
AT (0, 0, 0) ABSOLUTE
```

McStasScript

Quick demo

- Parameter objects
- Calculations
- Parameter overview



```
src.lambda0 = instrument.add_parameter("wavelength", value=5.0, comment="Wavelength [AA]")
src.dlambda = "0.1*wavelength"
print(src)

COMPONENT source = Source_div(
    xwidth = 0.1, // [m]
    yheight = 0.05, // [m]
    focus_aw = 1.2, // [deg]
    focus_ah = 2.3, // [deg]
    lambda0 = wavelength, // [Ang]
    dlambda = 0.1*wavelength // [Ang]
)
AT (0, 0, 0) ABSOLUTE

instrument.show_parameters()

wavelength = 5.0 // Wavelength [AA]
```

McStasScript

Quick demo

- Set position
- For-loop



python™



```
guide = instrument.add_component("extraction", "Guide_gravity")
guide.set_parameters(w1=0.05, h1=0.05, l=4.0, m=3.5, G=-9.82)
guide.set_AT([0,0,2], RELATIVE=src)
```

```
last_element = guide
for index in range(1, 6):
    guide = instrument.add_component("guide_" + str(index), "Guide_gravity")
    guide.set_parameters(w1=0.05, h1=0.05, l=1.0, m=3.5, G=-9.82)
    guide.set_AT(last_element.l + 1E-3, RELATIVE=last_element)
    guide.set_ROTATED([0, 0.3, 0], RELATIVE=last_element)

    last_element = guide
```

- Component list

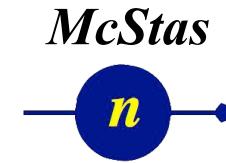
```
instrument.show_components()
```

source	Source_div	AT	(0, 0, 0)	ABSOLUTE
extraction	Guide_gravity	AT	(0, 0, 2)	RELATIVE source
guide_1	Guide_gravity	AT	(0, 0, 4.001)	RELATIVE extraction
		ROTATED	(0, 0.3, 0)	RELATIVE extraction
guide_2	Guide_gravity	AT	(0, 0, 1.001)	RELATIVE guide_1
		ROTATED	(0, 0.3, 0)	RELATIVE guide_1
guide_3	Guide_gravity	AT	(0, 0, 1.001)	RELATIVE guide_2
		ROTATED	(0, 0.3, 0)	RELATIVE guide_2
guide_4	Guide_gravity	AT	(0, 0, 1.001)	RELATIVE guide_3
		ROTATED	(0, 0.3, 0)	RELATIVE guide_3
guide_5	Guide_gravity	AT	(0, 0, 1.001)	RELATIVE guide_4
		ROTATED	(0, 0.3, 0)	RELATIVE guide_4

McStasScript

Quick demo

- Filename pitfall
- Diagrams

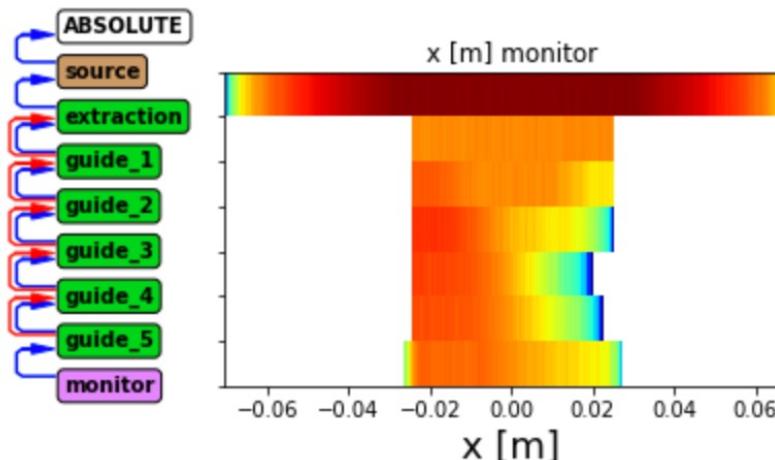
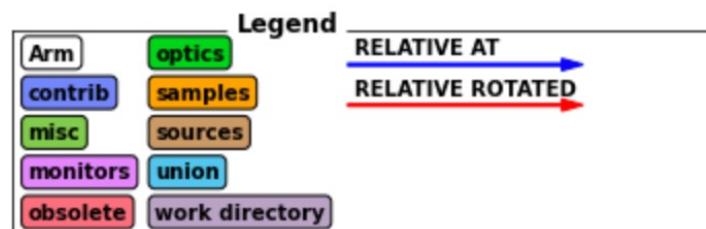


python™



```
mon = instrument.add_component("monitor", "PSD_monitor")
mon.set_parameters(nx = 100, ny = 100, filename = "psd.dat",
                    xwidth = 0.08, yheight = 0.08, restore_neutron = 1)
mon.set_AT([0,0,0.1 + guide.l], RELATIVE=guide)
```

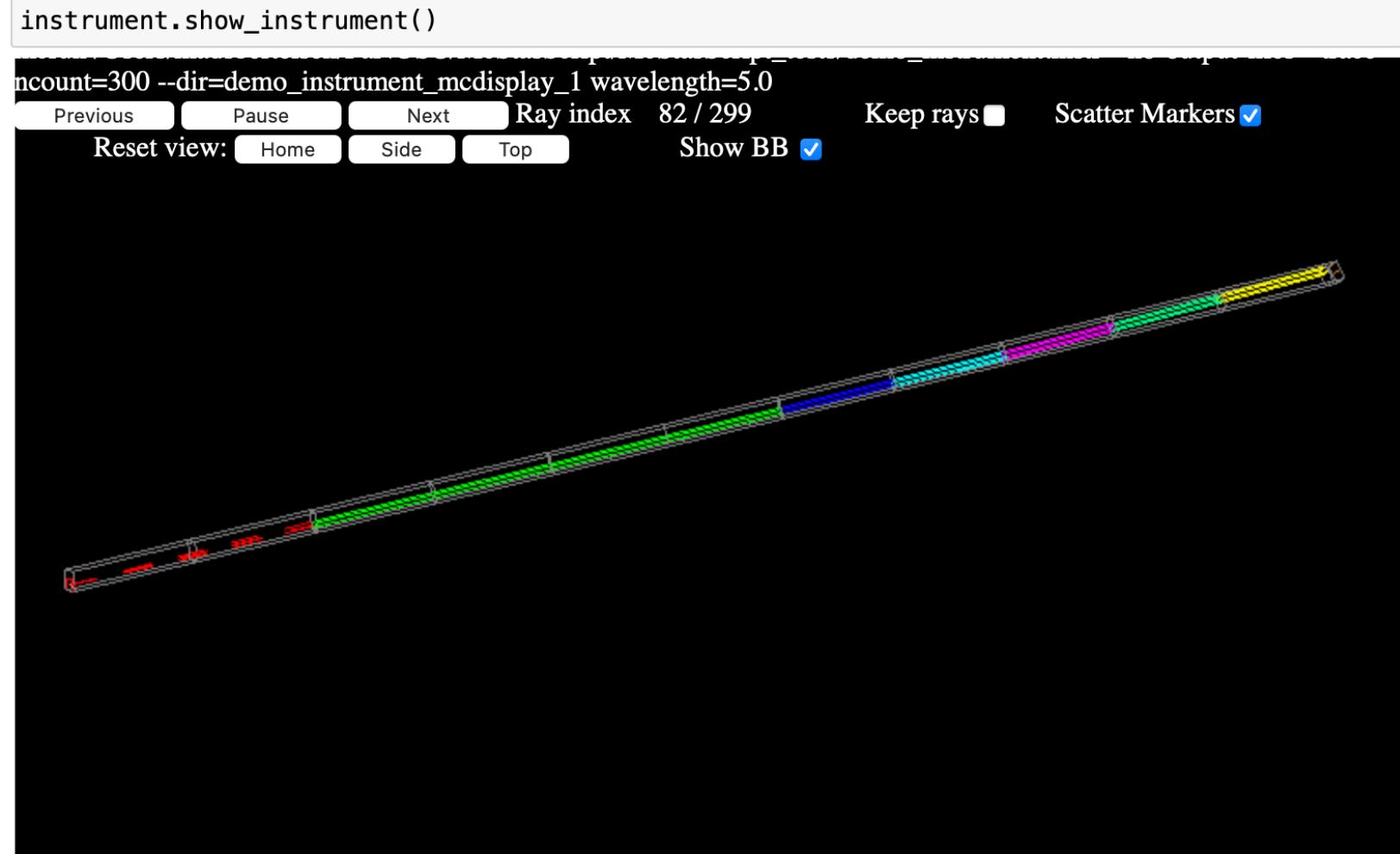
```
instrument.show_diagram(analysis=True, variable="x")
```



McStasScript

Quick demo

- Visualization



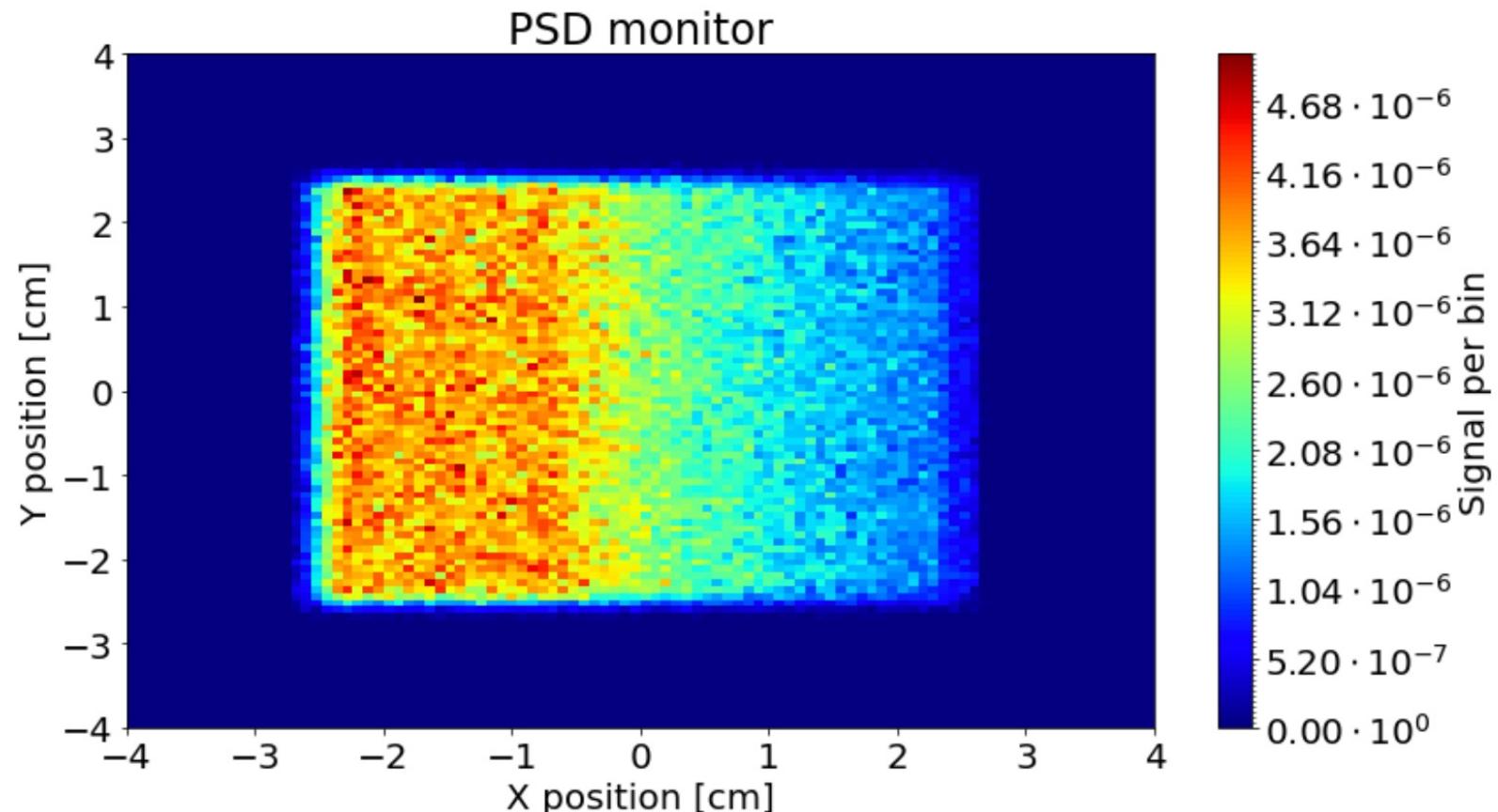
McStasScript

Quick demo

- Settings
- Parameters
- Run simulation
- Plot data

```
instrument.settings(ncount=1E6)
instrument.set_parameters(wavelength=5.0)
data = instrument.backengine()

ms.make_plot(data, fontsize=20)
```



McStasScript

Quick demo

- Python objects

- Metadata

- Numpy arrays



```
data
[
    McStasData: monitor type: 2D I:0.0106059 E:1.95751e-05 N:298700.0]
```

```
monitor = ms.name_search("monitor", data)
print(monitor.metadata)
```

```
metadata object
component_name: monitor
filename: psd.dat
2D data of dimension (100, 100)
    [-4.0: 4.0] X position [cm]
    [-4.0: 4.0] Y position [cm]
    Signal per bin
Instrument parameters:
    wavelength = 5.0
```

```
monitor.Intensity[20:28, 40:44]
```

```
array([[3.23134550e-06, 3.14453425e-06, 2.93890316e-06, 3.20877876e-06],
       [3.38387710e-06, 3.33175403e-06, 3.50741480e-06, 3.58799402e-06],
       [3.55206636e-06, 4.25656257e-06, 3.73936568e-06, 3.76360681e-06],
       [3.87306679e-06, 2.86940652e-06, 3.28559204e-06, 3.16032605e-06],
       [4.09563983e-06, 3.77835214e-06, 3.47772083e-06, 2.82467245e-06],
       [3.86452494e-06, 3.40783311e-06, 3.92903001e-06, 4.12164357e-06],
       [3.20800343e-06, 3.72103256e-06, 3.26505458e-06, 3.65186330e-06],
       [3.18478308e-06, 3.86097677e-06, 3.37923228e-06, 3.49790361e-06]])
```

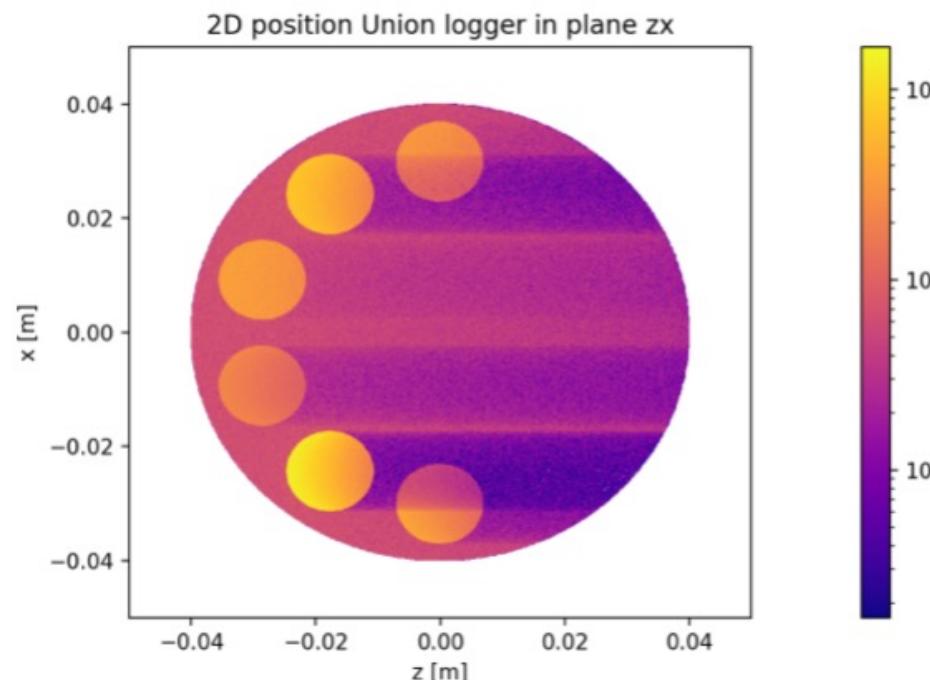
McStasScript

Quick demo

- Simulation widget

energy	10.0	[meV] Energy of source
delta_energy	8.0	[meV] Energy spread of source
rotation_y	180.0	[deg] Rotation around vertical
rotation_x	0.0	[deg] Rotation around horizontal
material	"Pb"	Material choice for extra material sample
<input type="button" value="Run"/> ncount 1E8 mpi 4		

Figure 1



Choose monitor

Plot options

Log plot

Orders of magnitude

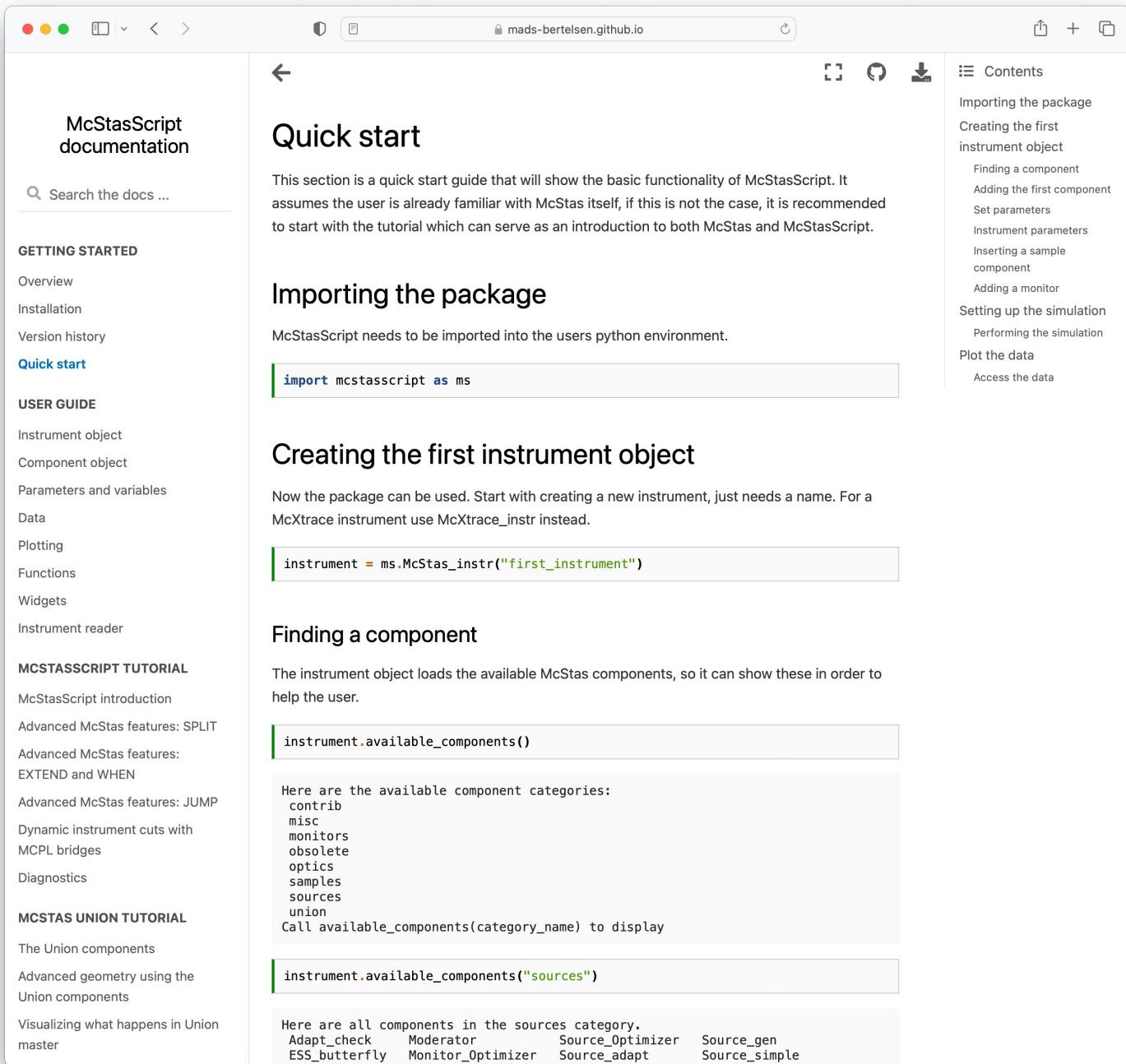
Colormap category

Colormap

McStasScript

Documentation

- Comprehensive documentation
- Descriptions of the classes
- Tutorials for
 - McStasScript
 - McStas features
 - McStas Union components
- <https://mads-bertelsen.github.io>
- Workshop / School available



The screenshot shows a web browser displaying the McStasScript documentation at <https://mads-bertelsen.github.io>. The page has a sidebar with navigation links and a search bar. The main content area includes sections for 'Quick start', 'Importing the package', 'Creating the first instrument object', 'Finding a component', and code snippets illustrating how to use the package.

McStasScript documentation

Search the docs ...

GETTING STARTED

- Overview
- Installation
- Version history
- Quick start**

USER GUIDE

- Instrument object
- Component object
- Parameters and variables
- Data
- Plotting
- Functions
- Widgets
- Instrument reader

MCSTASSCRIPT TUTORIAL

- McStasScript introduction
- Advanced McStas features: SPLIT
- Advanced McStas features: EXTEND and WHEN
- Advanced McStas features: JUMP
- Dynamic instrument cuts with MCPL bridges
- Diagnostics

MCSTAS UNION TUTORIAL

- The Union components
- Advanced geometry using the Union components
- Visualizing what happens in Union master

Quick start

This section is a quick start guide that will show the basic functionality of McStasScript. It assumes the user is already familiar with McStas itself, if this is not the case, it is recommended to start with the tutorial which can serve as an introduction to both McStas and McStasScript.

Importing the package

McStasScript needs to be imported into the users python environment.

```
import mcstasscript as ms
```

Creating the first instrument object

Now the package can be used. Start with creating a new instrument, just needs a name. For a McXtrace instrument use McXtrace_instr instead.

```
instrument = ms.McStas_instr("first_instrument")
```

Finding a component

The instrument object loads the available McStas components, so it can show these in order to help the user.

```
instrument.available_components()
```

Here are the available component categories:

```
contrib
misc
monitors
obsolete
optics
samples
sources
union
```

Call `available_components(category_name)` to display

```
instrument.available_components("sources")
```

Here are all components in the sources category.

```
Adapt_check Moderator Source_Optimizer Source_gen
ESS_butterfly Monitor_Optimizer Source_adapt Source_simple
ESS_dipole Monitor_Threshold Source_dipole Source_threshold
```

Contents

- Importing the package
- Creating the first instrument object
 - Finding a component
 - Adding the first component
 - Set parameters
 - Instrument parameters
 - Inserting a sample component
 - Adding a monitor
- Setting up the simulation
 - Performing the simulation
 - Plot the data
- Access the data

Timeline Overview

University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



Position



Subject



Software



guide_bot

Python version

- HighNESS project
- Rewrite of guide_bot in Python
- Easier to ...
 - Install
 - Expand
 - Use
- No license, more powerful
- Uses McStasScript

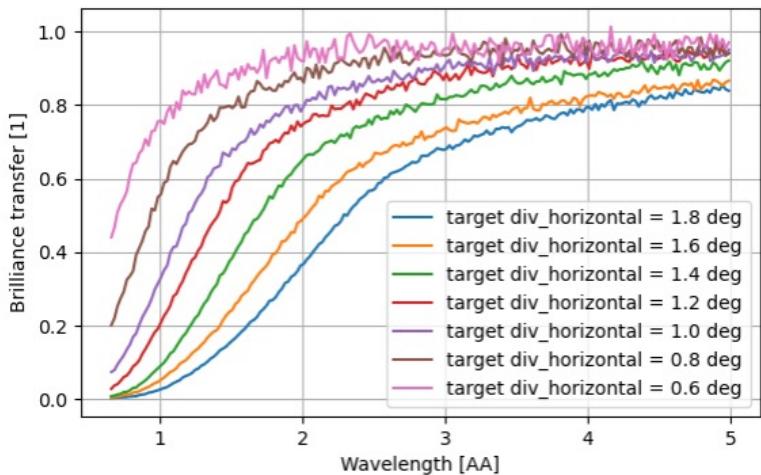
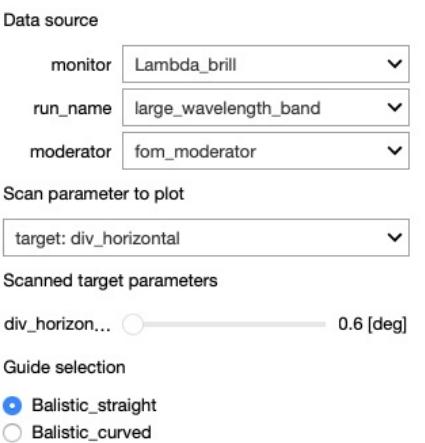
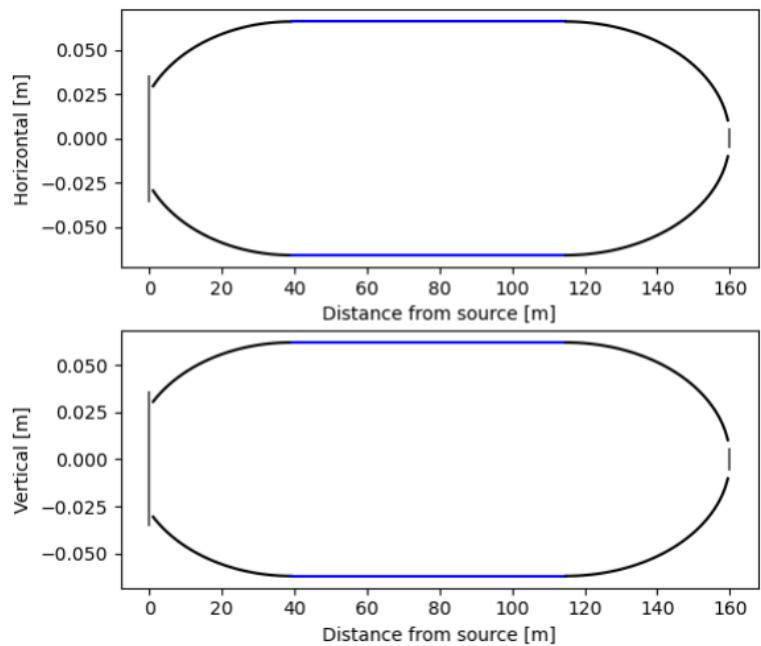
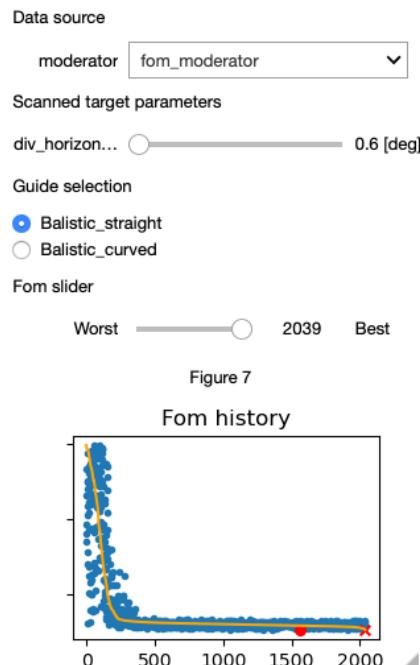
guide_bot project

```
target = gb.Target(width=0.01, height=[0.02, 0.04, 0.06],  
                   div_horizontal=0.75, div_vertical=1.2,  
                   min_wavelength=1.5, max_wavelength=3.0,  
                   instrument_length=60, target_guide_distance=0.5)  
  
moderator = gb.Moderator(name="fom_moderator", guide_start=2.0,  
                           width=0.1, height=0.05)  
  
highness = gb.MCPL_source(name="3x3", mcpl_file="3x3.mcpl",  
                           width=0.03, height=0.03)  
  
project = gb.Project(name="demo",  
                     target=target, moderator=moderator,  
                     analysis_moderators=highness)  
  
guide = project.new_guide(name="feeder_and_curved")  
guide += gb.Elliptic(name="Feeder")  
guide += gb.Gap(name="Chopper_gap", start_point=6.5,  
                start_width=0.03, start_height=0.05)  
guide += gb.Curved(name="Curved", start_point=6.6)  
guide += gb.Elliptic(name="Focusing")  
  
project.write(cluster=DMSC)
```

guide_bot

Python version

- HighNESS project
- Rewrite of guide_bot in Python
- Easier to ...
 - Install
 - Expand
 - Use
- No license, more powerful
- Uses McStasScript
- Nice widgets for visualization



Timeline Overview

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European Spallation Source



My work with McStas



Position



Subject

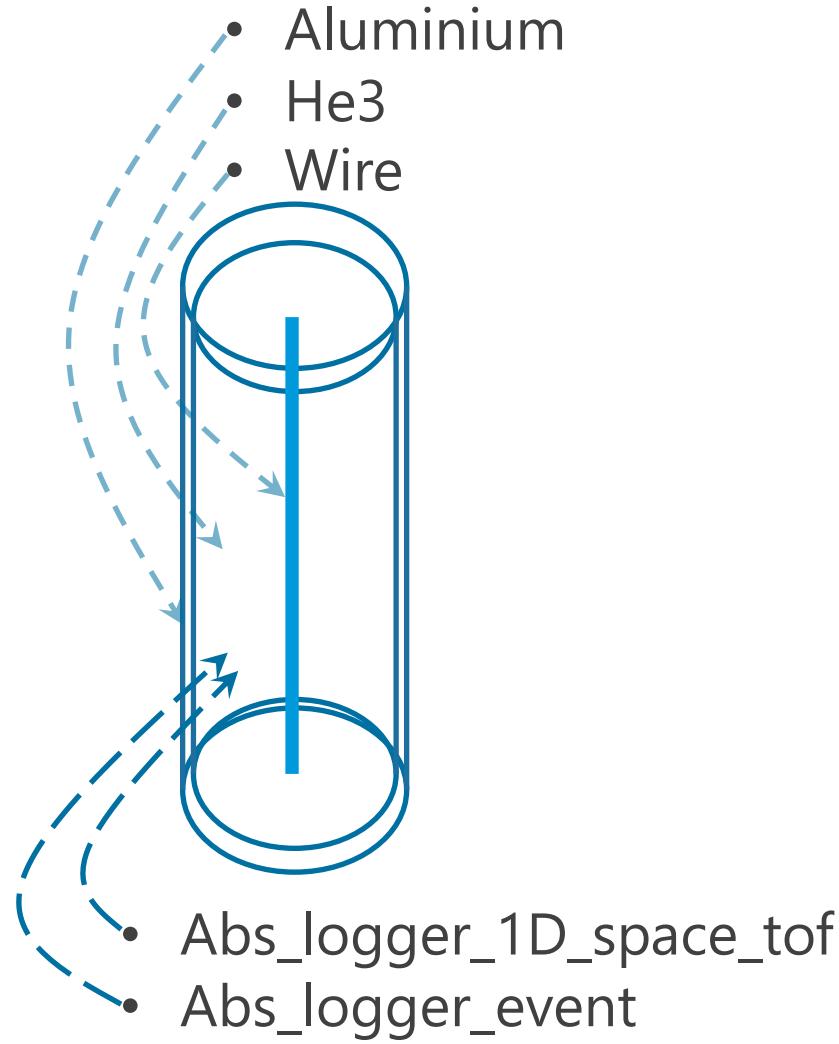


Software

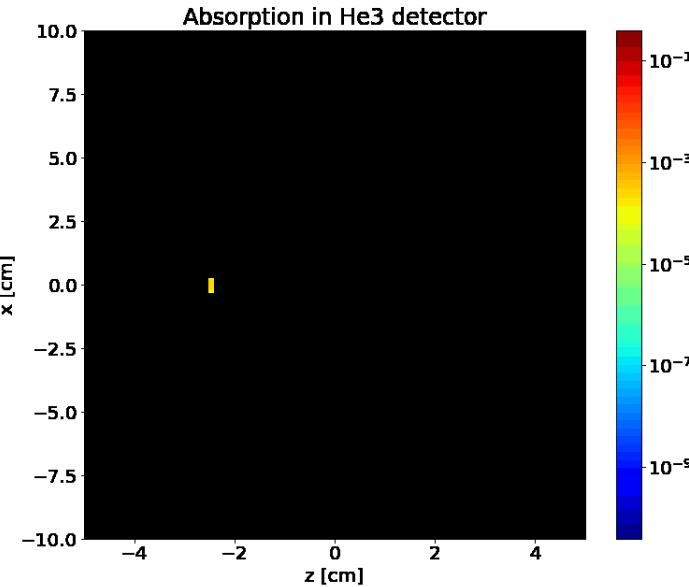


Detectors

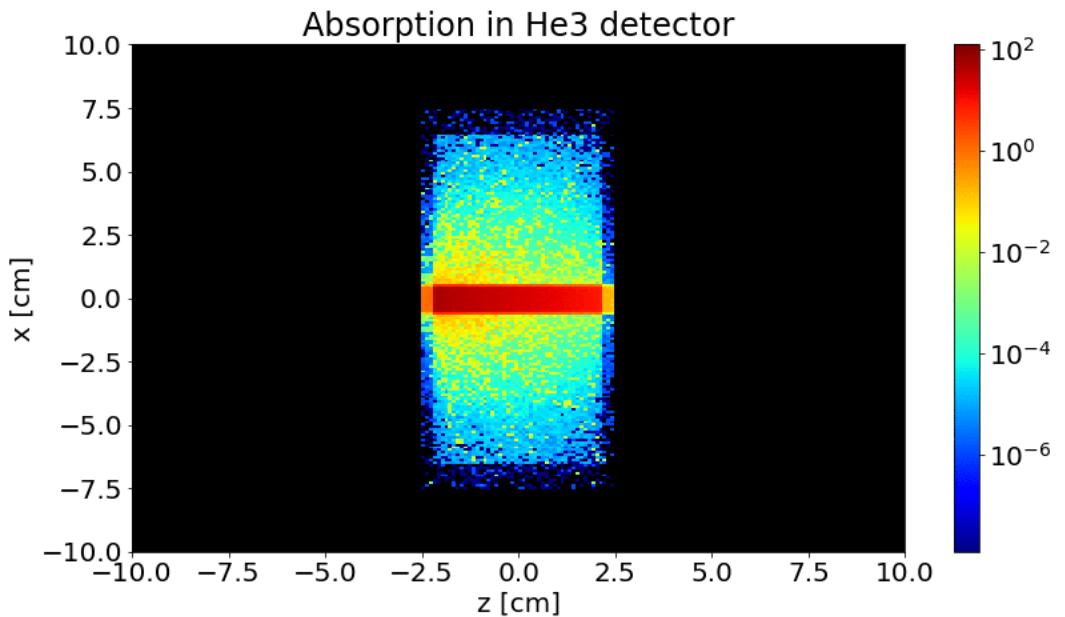
Overview



Small wavelength interval

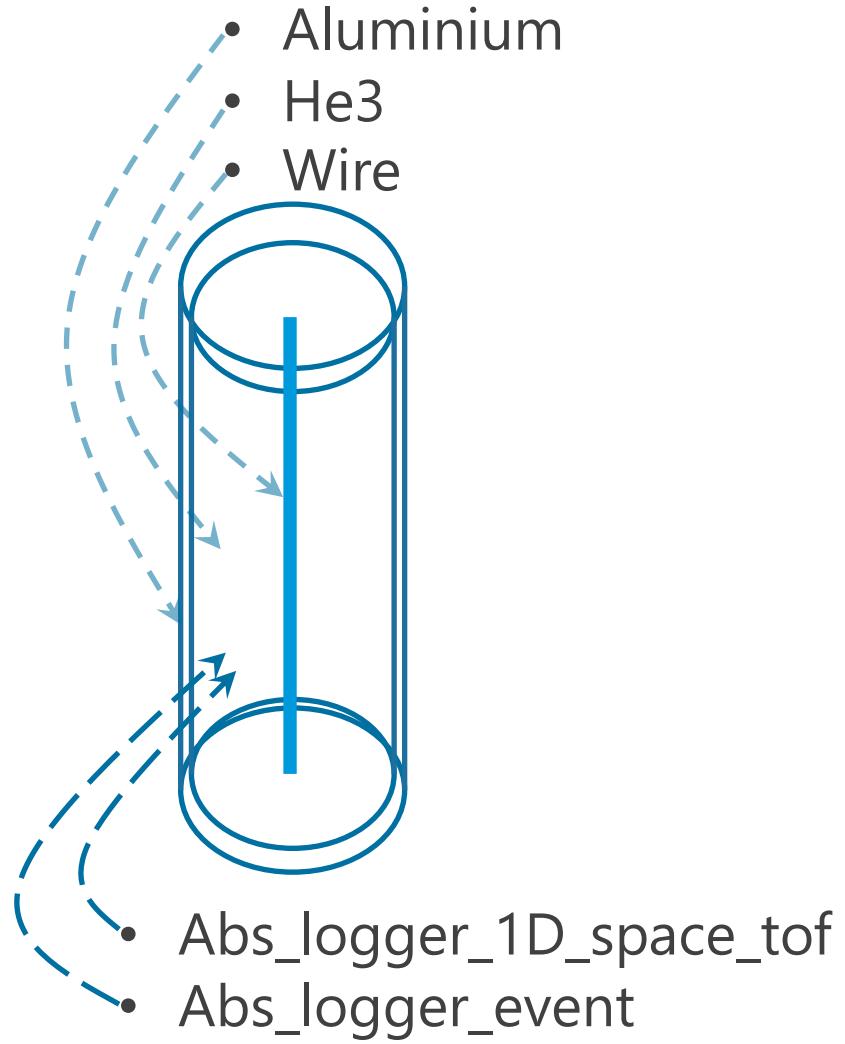


Large wavelength interval

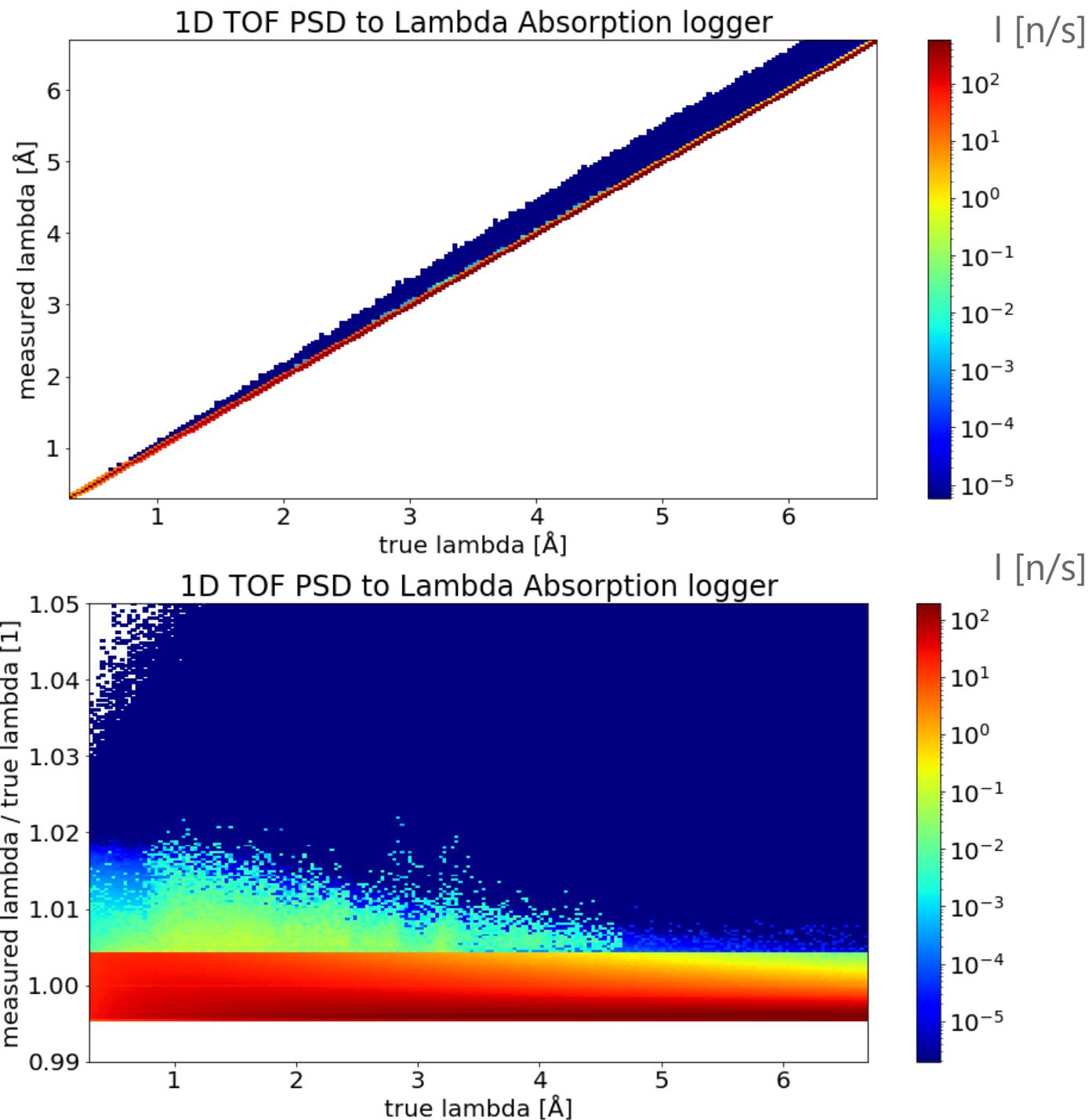


Detectors

Overview



2023-10-10



ENSA Award



The European Neutron Scattering Association - ENSA

awards the 2021

Neutron Instrumentation and Innovation Award

sponsored by Mirrotron
to

DR. MADS BERTELSEN

in recognition of his original contributions to extending capabilities of the neutron ray-tracing package McStas in particular by authoring the packages Guide-bot and Union, and for his work towards making these tools efficient to use by the community, which has already impacted design of many new instruments across different facilities.

Awarded at ICNS 2021 in Buenos Aires, August 23rd 2022,



President of ENSA
Prof. Henrik M. Rønnow

A handwritten signature in blue ink, appearing to read "Henrik Rønnow".

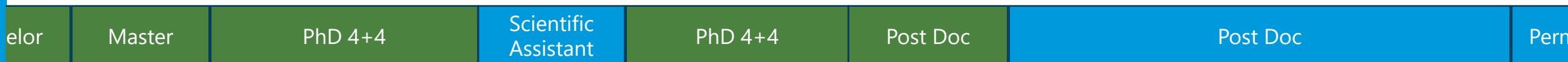
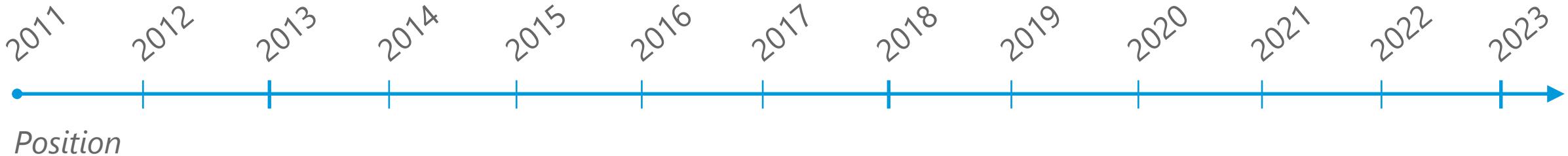
F. Jensen
MIRROTRON

Timeline Overview

University of Copenhagen - Kim Lefmann
European Spallation Source



My work with McStas



Subject



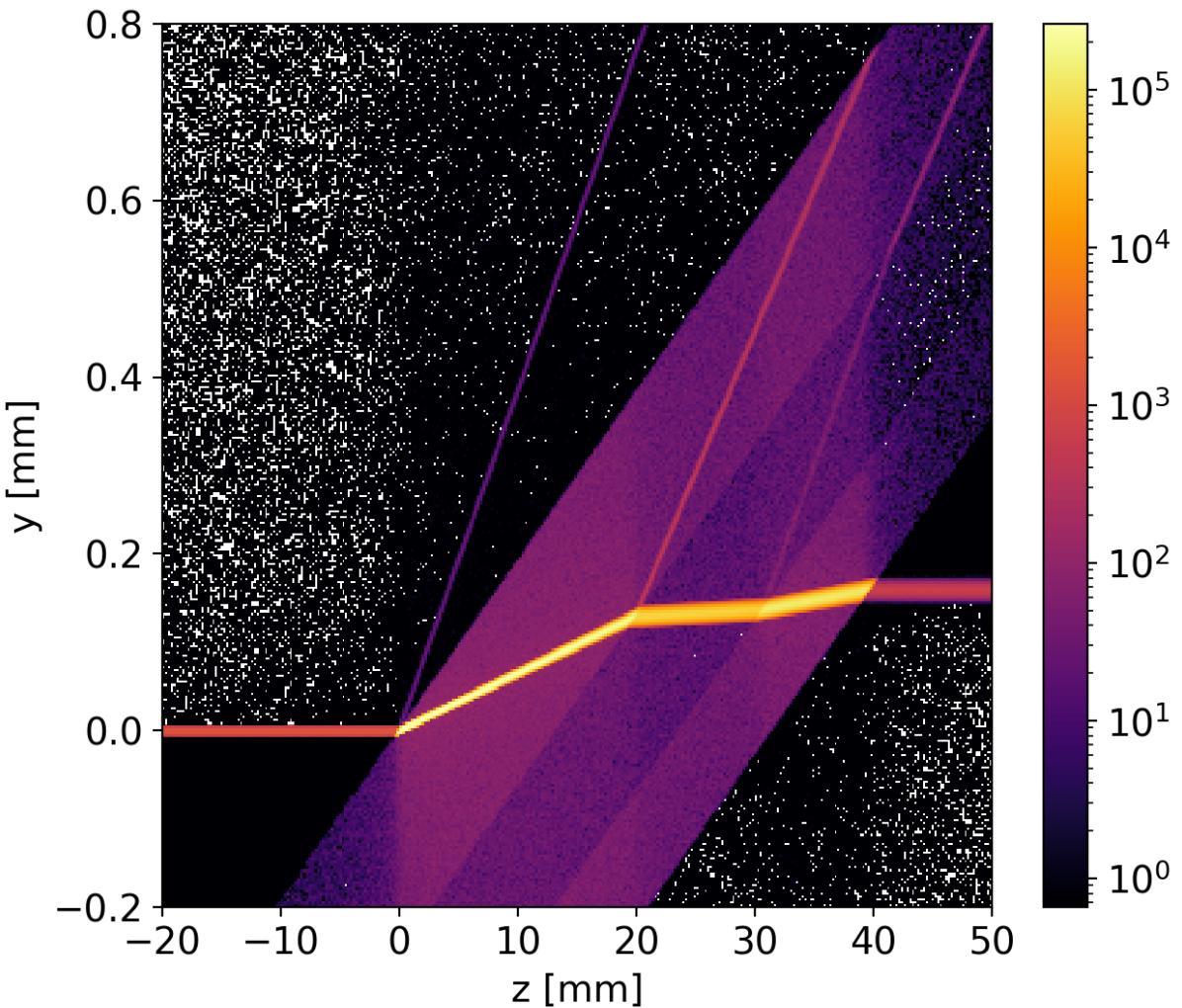
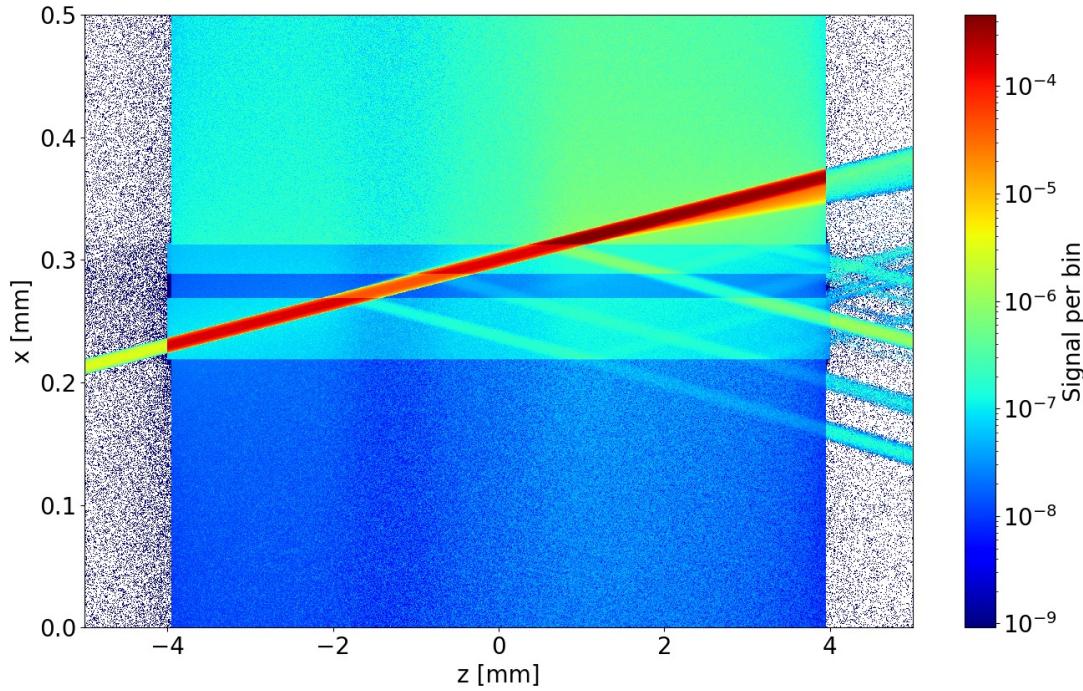
Software



Outlook

Union features

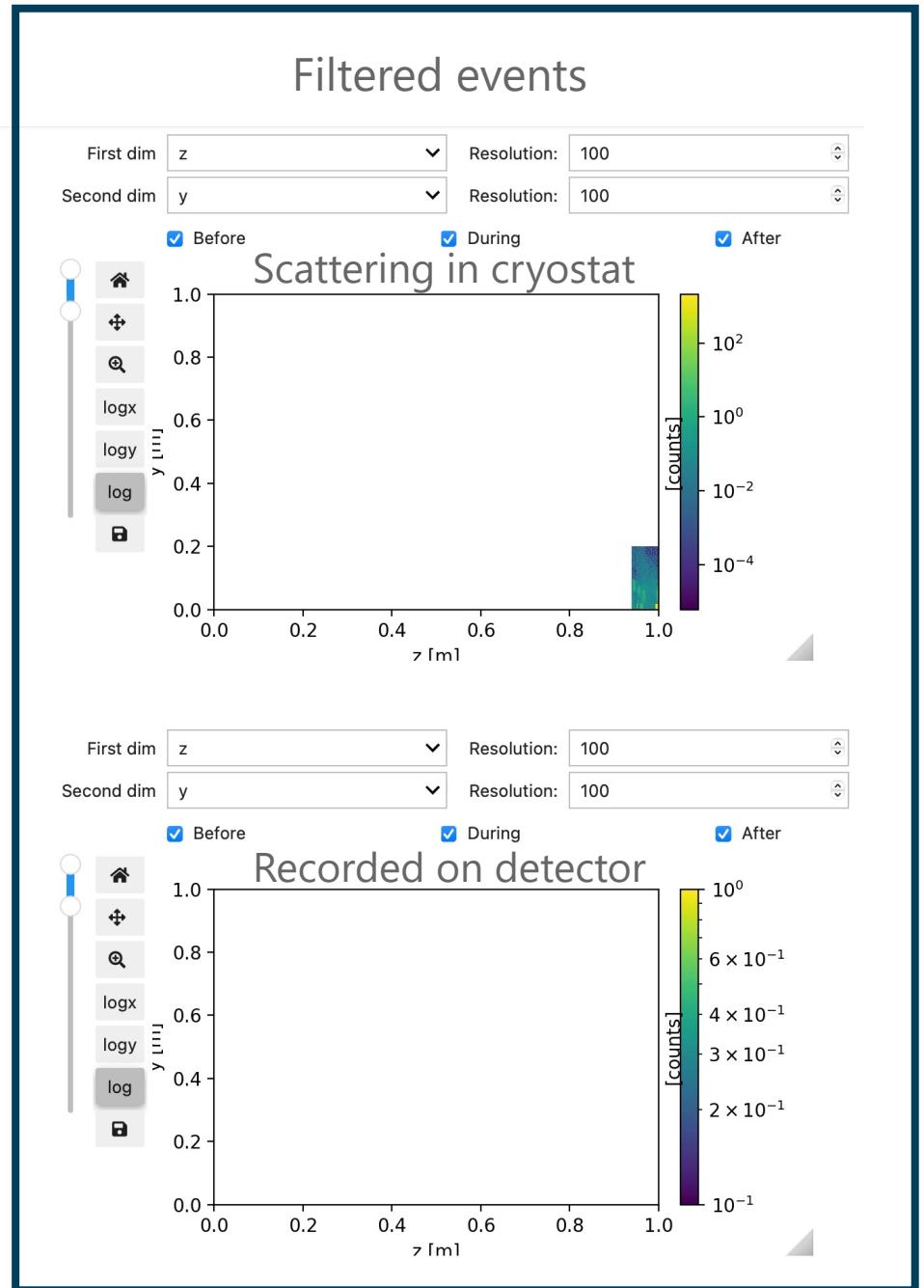
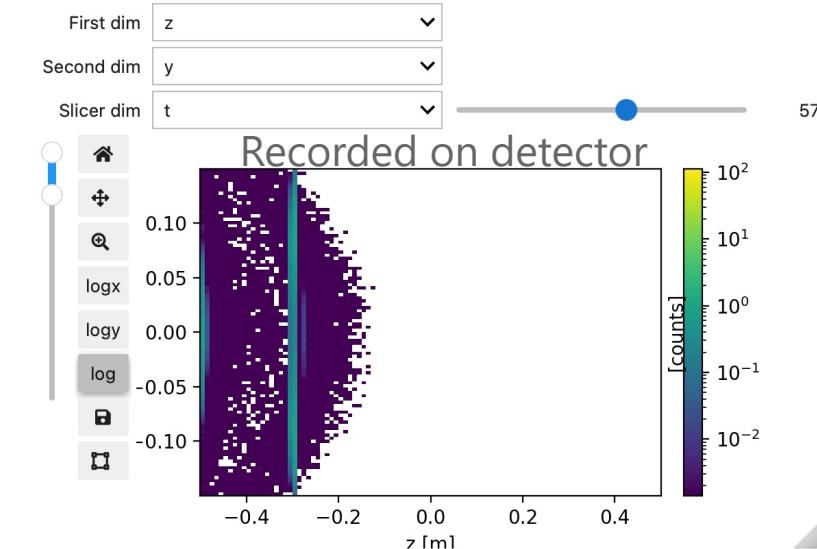
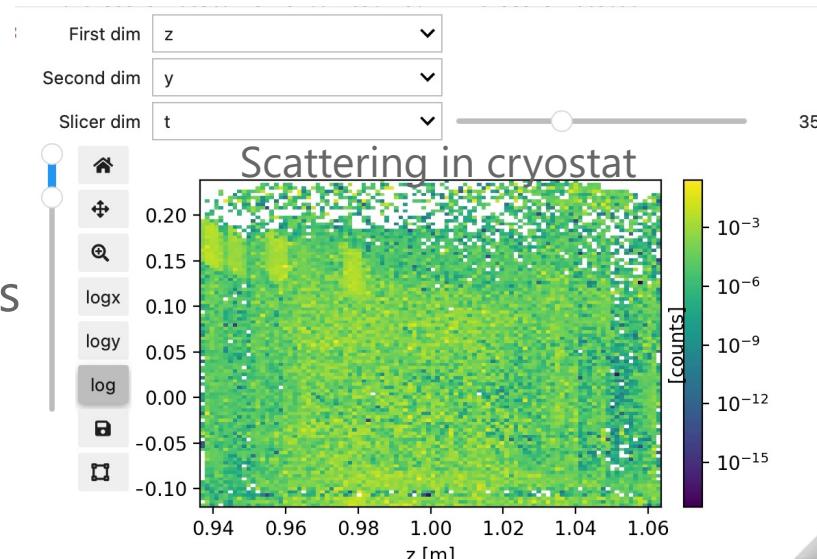
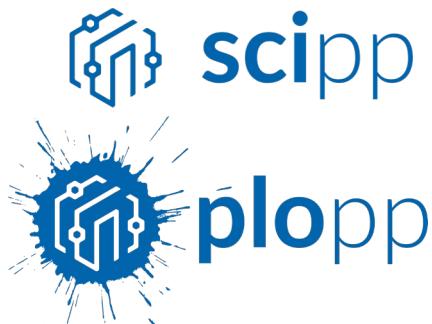
- Refraction in Union components
- Surface effects in general



Outlook

Widget

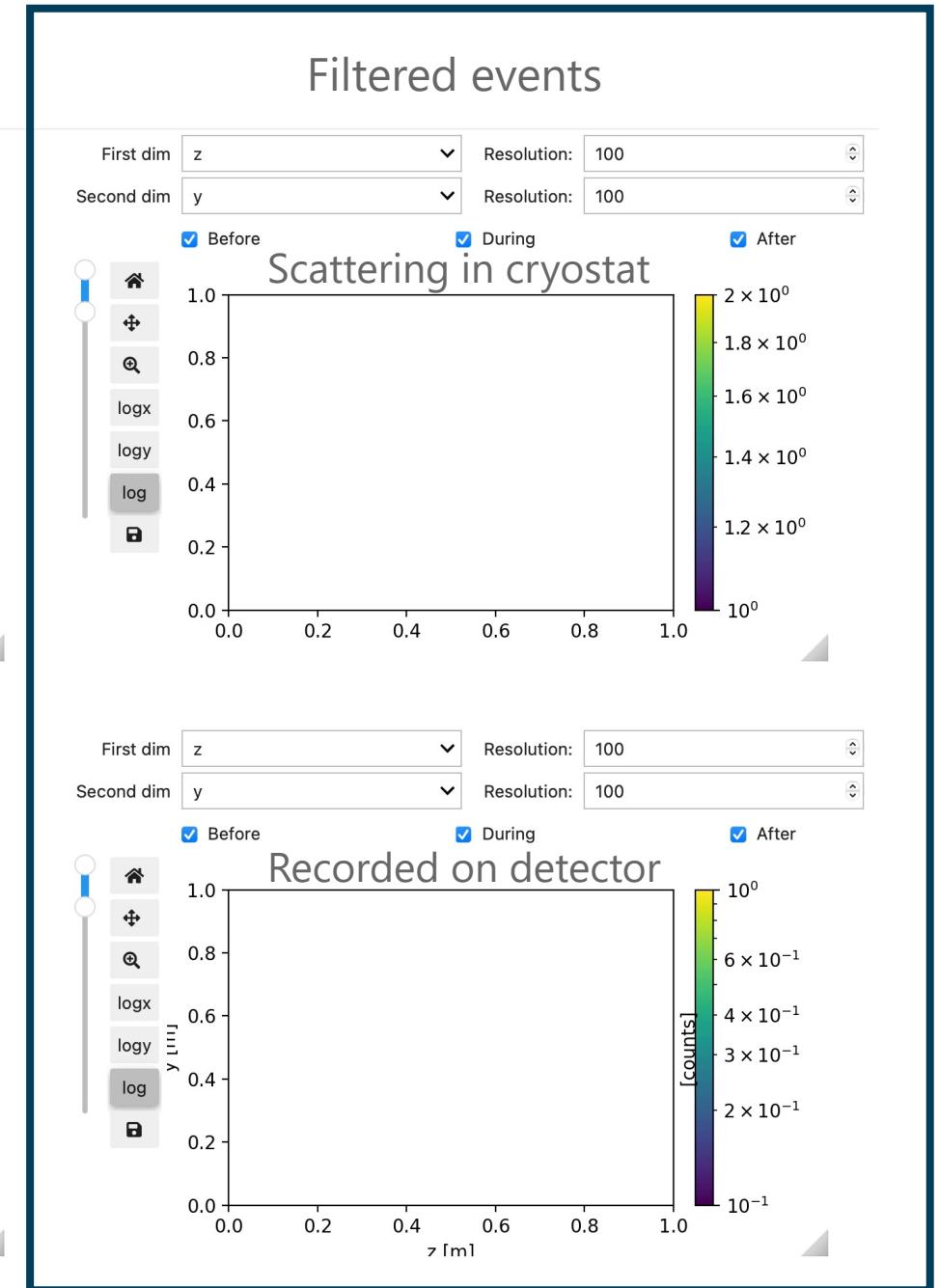
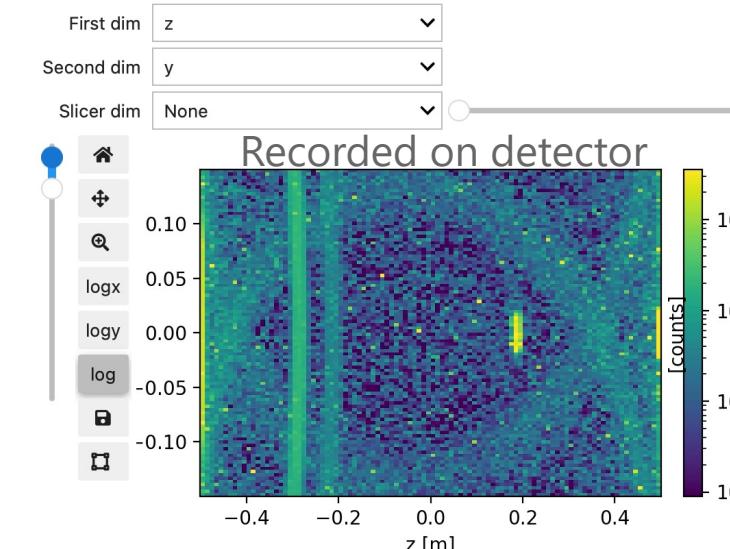
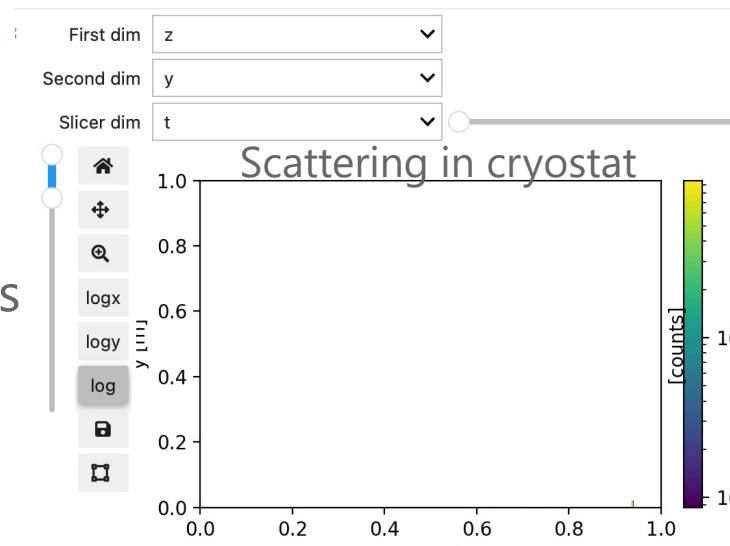
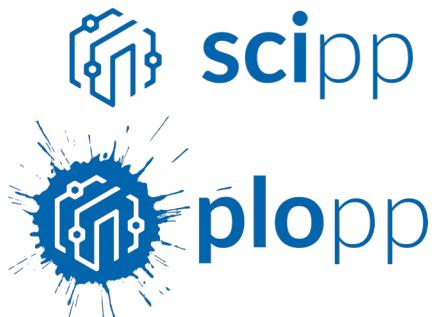
- Event data widget
- Explore ray histories



Outlook

Widget

- Event data widget
- Explore ray histories



Conclusion



- Seems it is possible to be a support scientist with simulation focus!
- My gratitude to all that have enabled me to be on this McStas journey
 - All developers of the software, especially Peter Willendrup
 - University supervisor Kim Lefmann
 - Wonderful colleagues at University of Copenhagen and at ESS



Thanks for your attention