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

Mads Bertelsen

McStas 25th Anniversary, 1998 - 2023

2023-10-10

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."

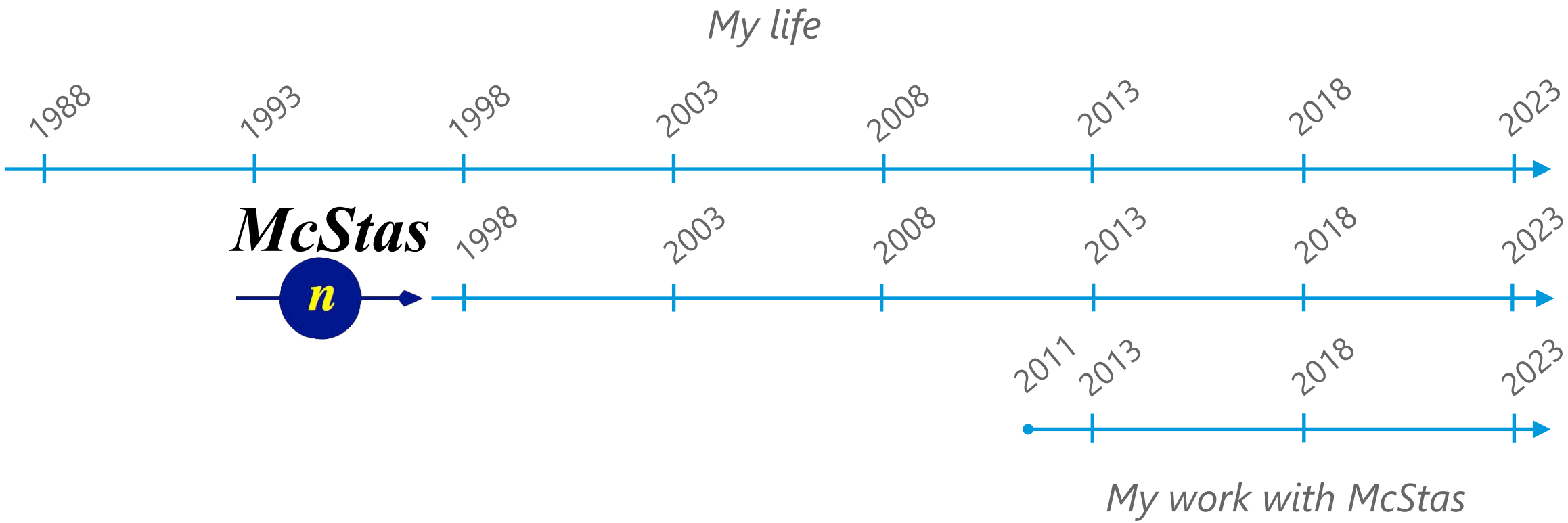
I think there is space for support scientists

Timeline

Overview

Timeline

Overview



Timeline

Overview

My work with McStas

Timeline

Overview

University of Copenhagen - Kim Lefmann

European Spallation Source

My work with McStas

Position

elor | Master | PhD 4+4

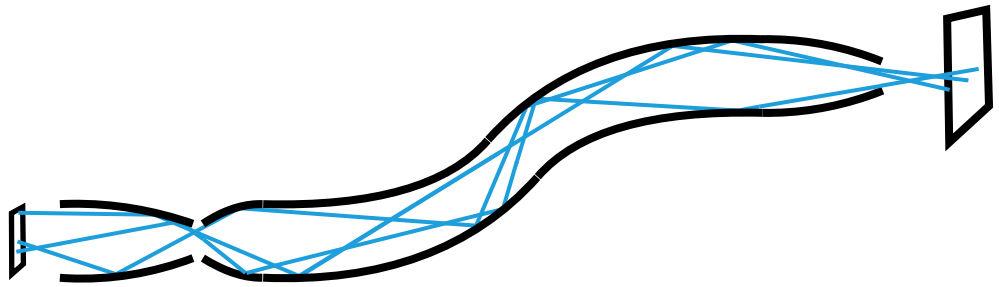
Subject

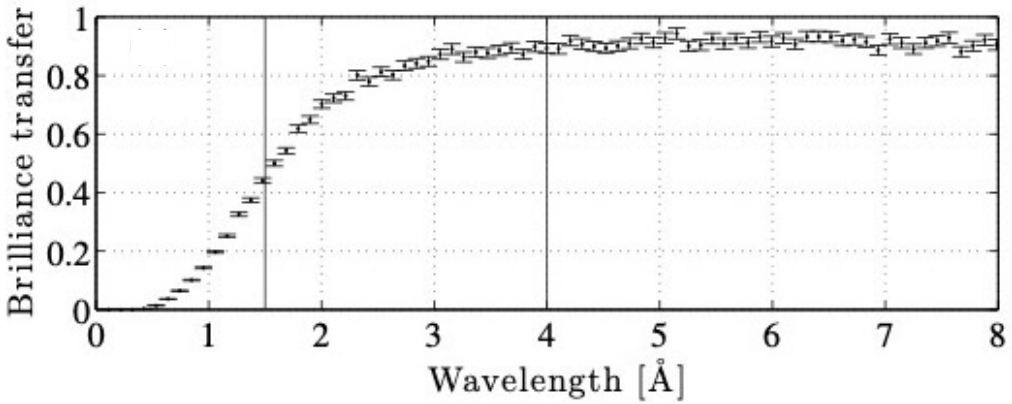
Moderators | Neutron optics

Guide design

A repetitive task

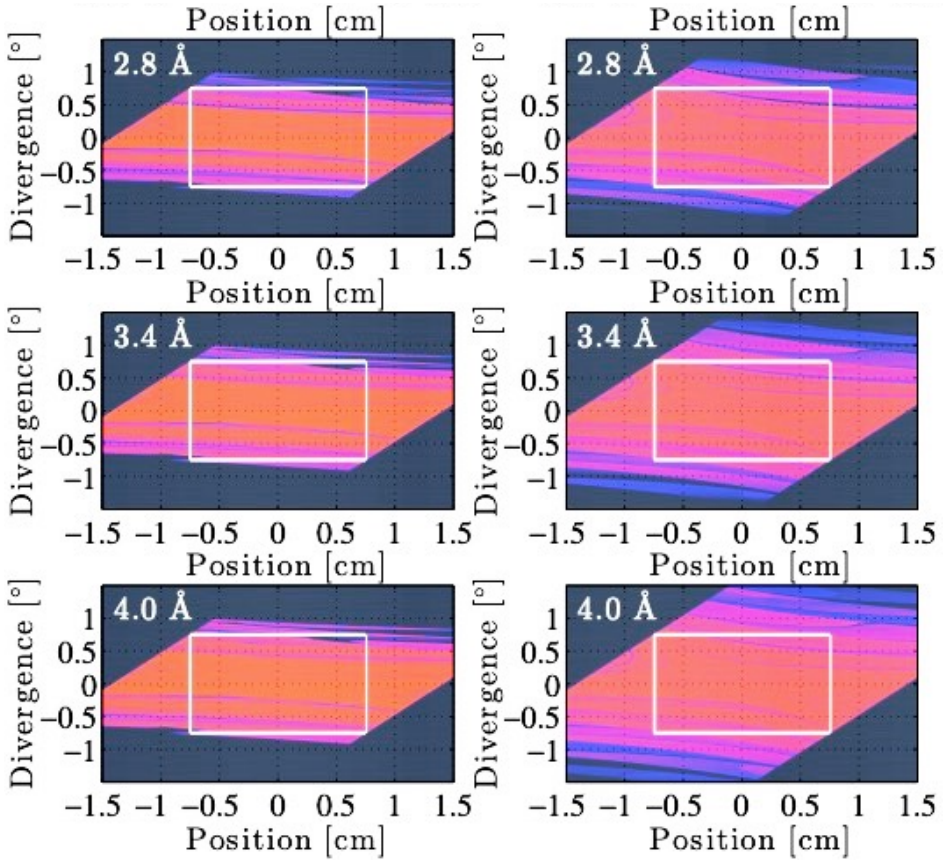
- Iterations of beam requirements
- Frequent rule changes from ESS
- Optimization for brilliance transfer with MATLAB + iFit
- Minimalist principle





Minimalist

No constraints



Timeline

Overview

University of Copenhagen - Kim Lefmann

European Spallation Source

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Subject

Moderators | Neutron optics

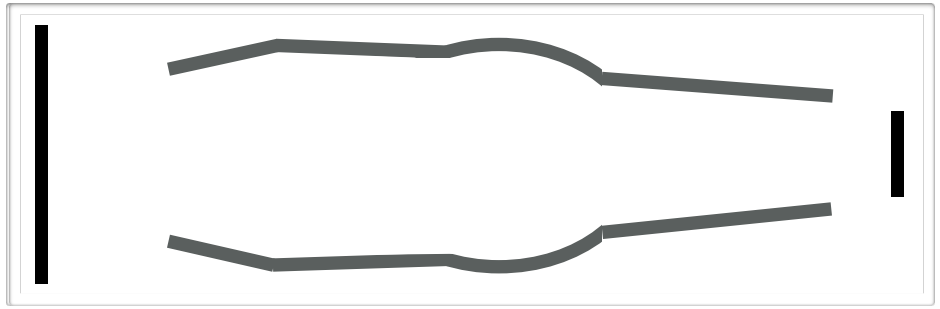
Software

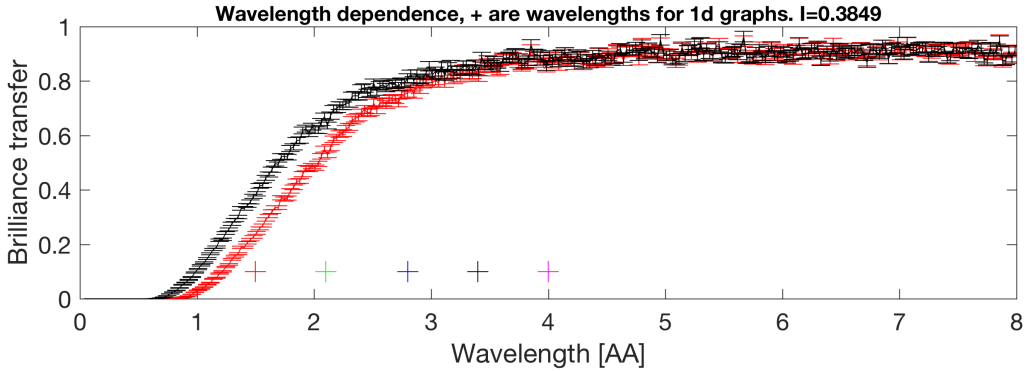
guide_bot MATLAB

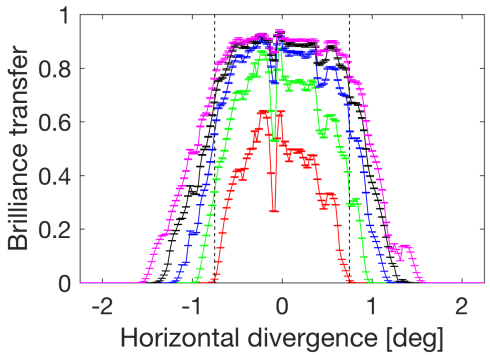
guide_bot

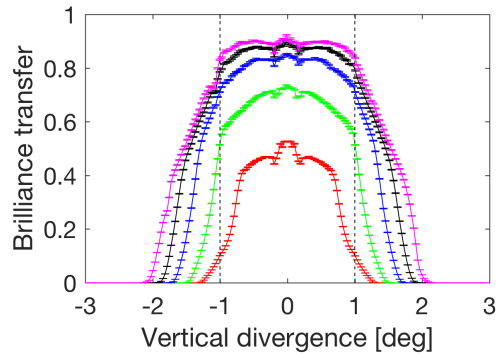
MATLAB Version

- 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









guide_bot

MATLAB Version

- Optimization of neutron guides
- Simple input for
  - Beam requirements
  - Source
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- Automated steps
  - Builds McStas simulations
  - Performs numerical optimization (iFit)
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- ESS
  - BIFROST
  - HEIMDAL
  - MIRACLES
  - VESPA
  - ESPRESSO
- PSI
  - CAMEA
  - FOCUS

Timeline

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elor | Master | PhD 4+4 | Scientific Assistant

Subject

Moderators | Neutron optics | Moderator - Optics coupling

Software

guide_bot MATLAB

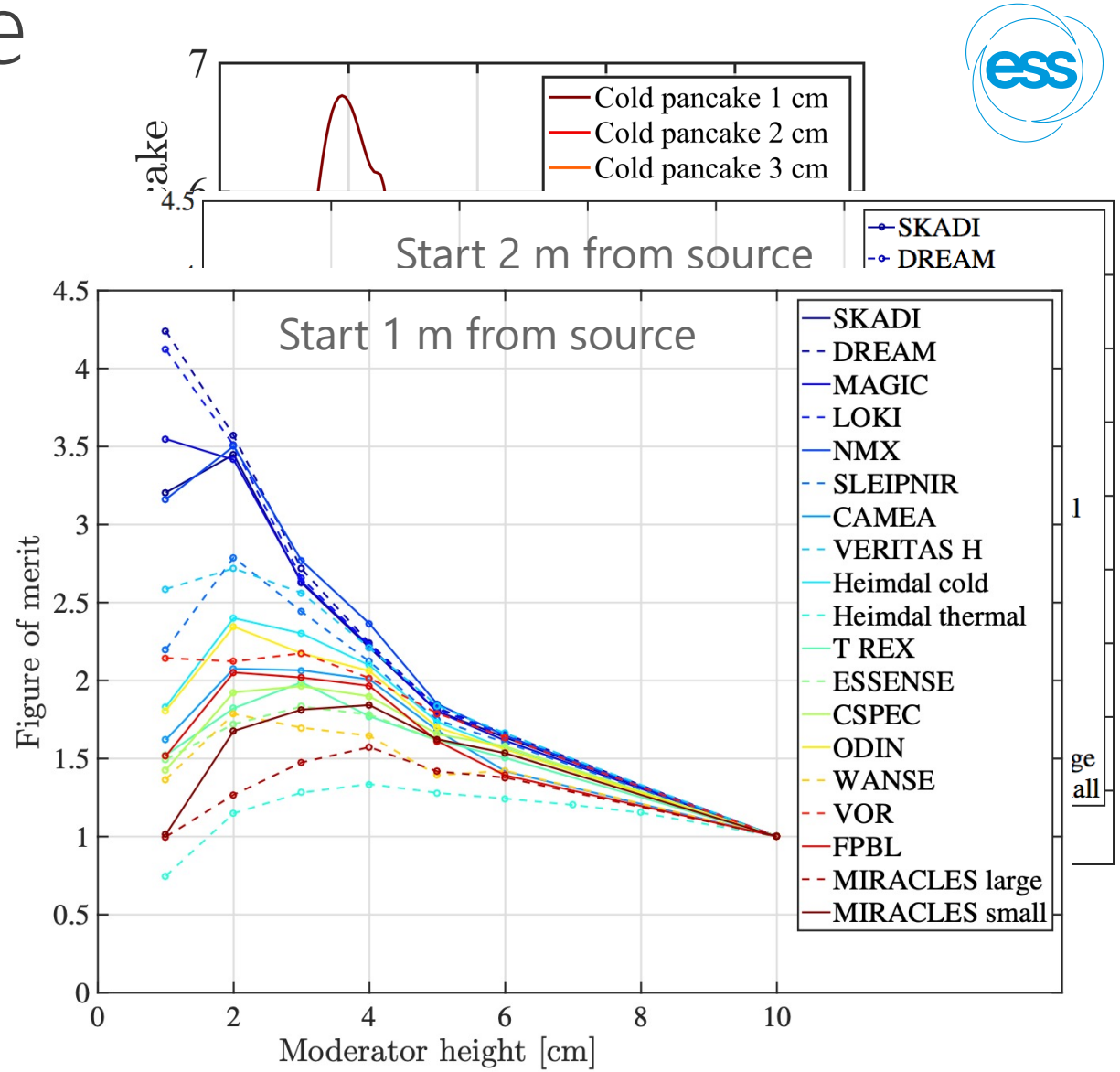
Job description

"Investigate pancakes and doughnuts."

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



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Subject

Moderators | Neutron optics | Moderator - Optics coupling | Samples | Sample environments + Instrument backends

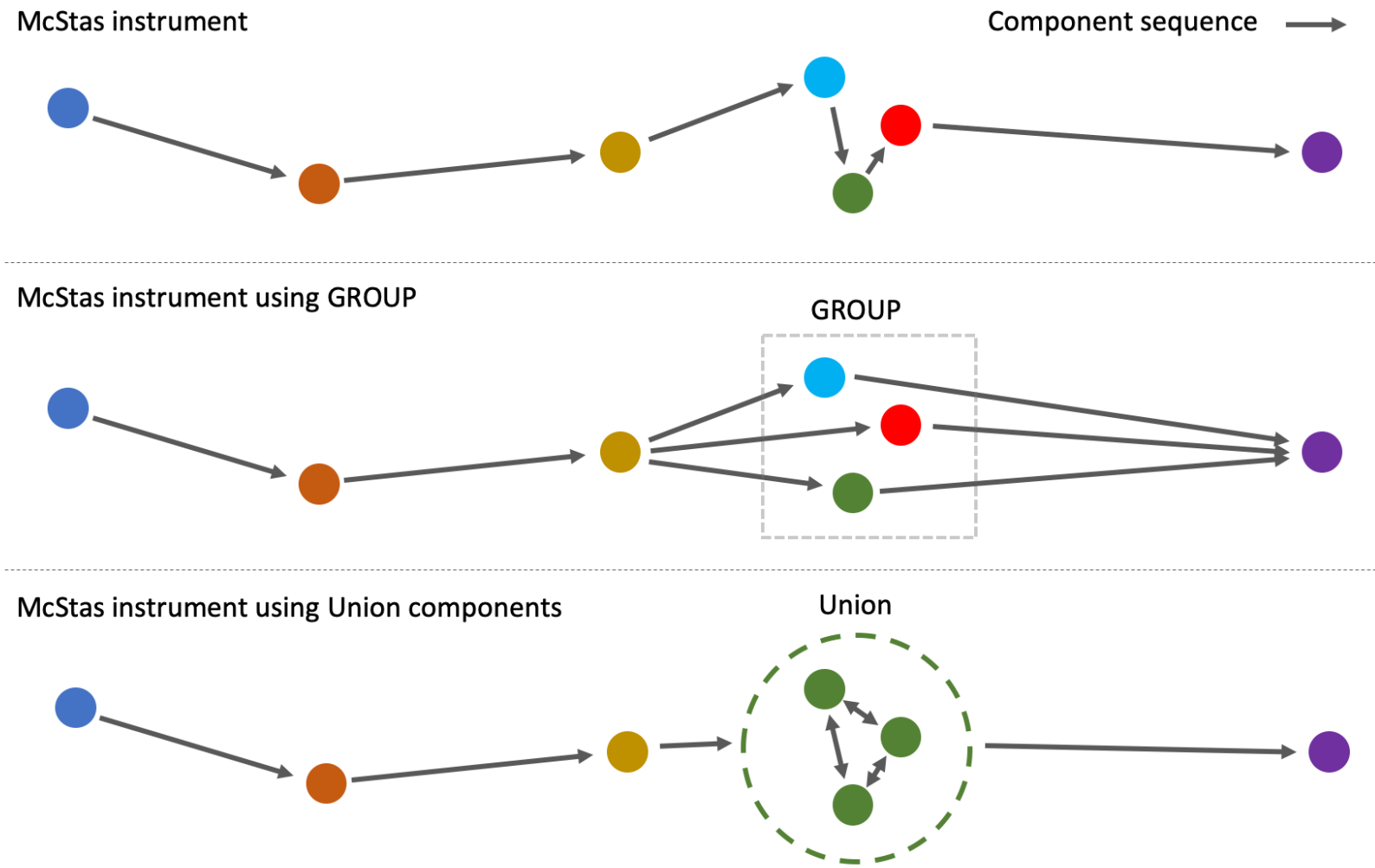
Software

guide_bot MATLAB

McStas Union components

Union components

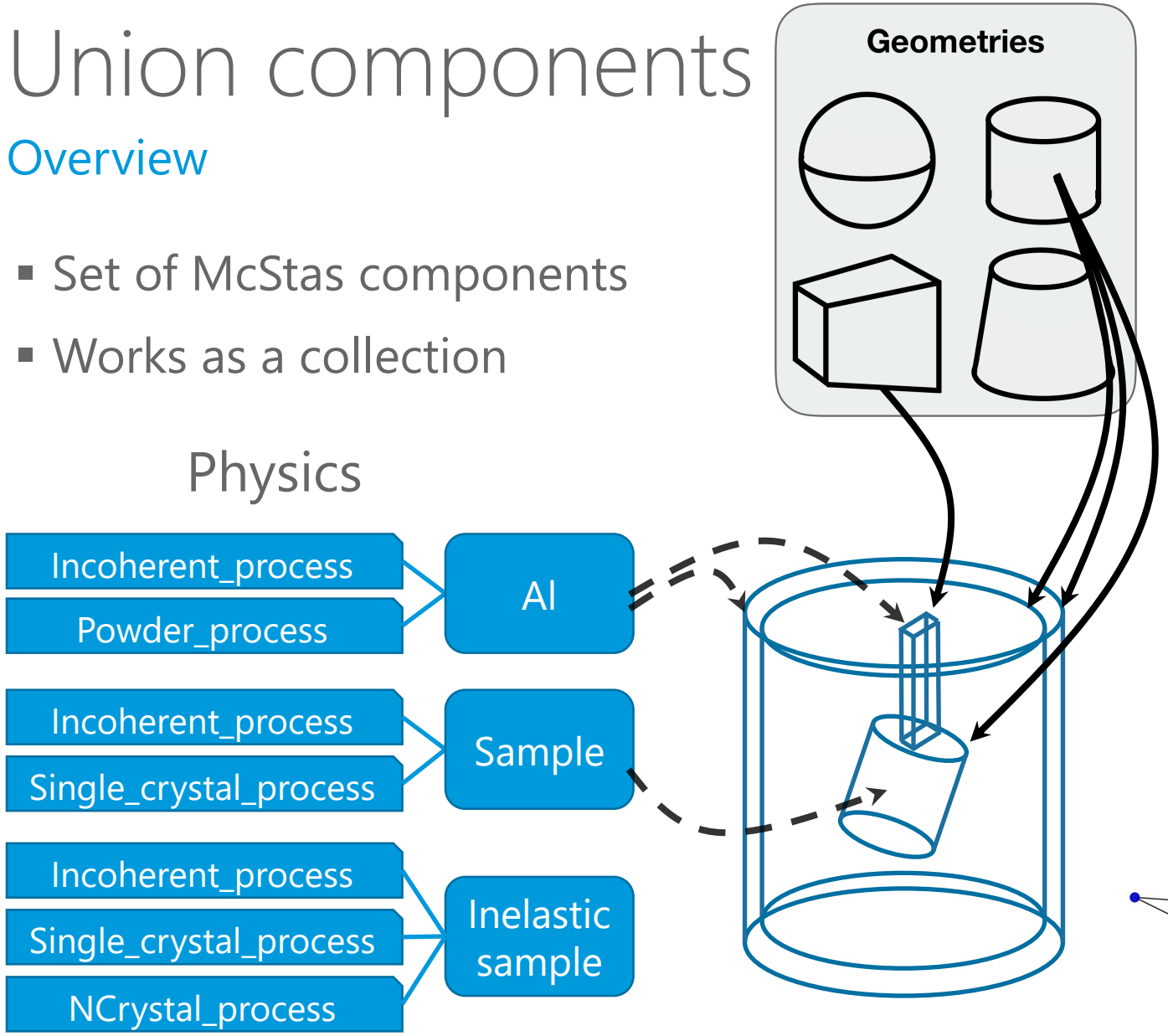
Union in the instrument

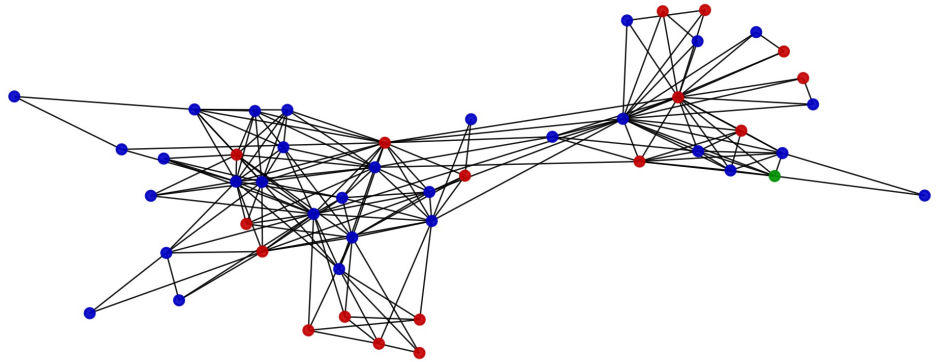


Union components

Overview

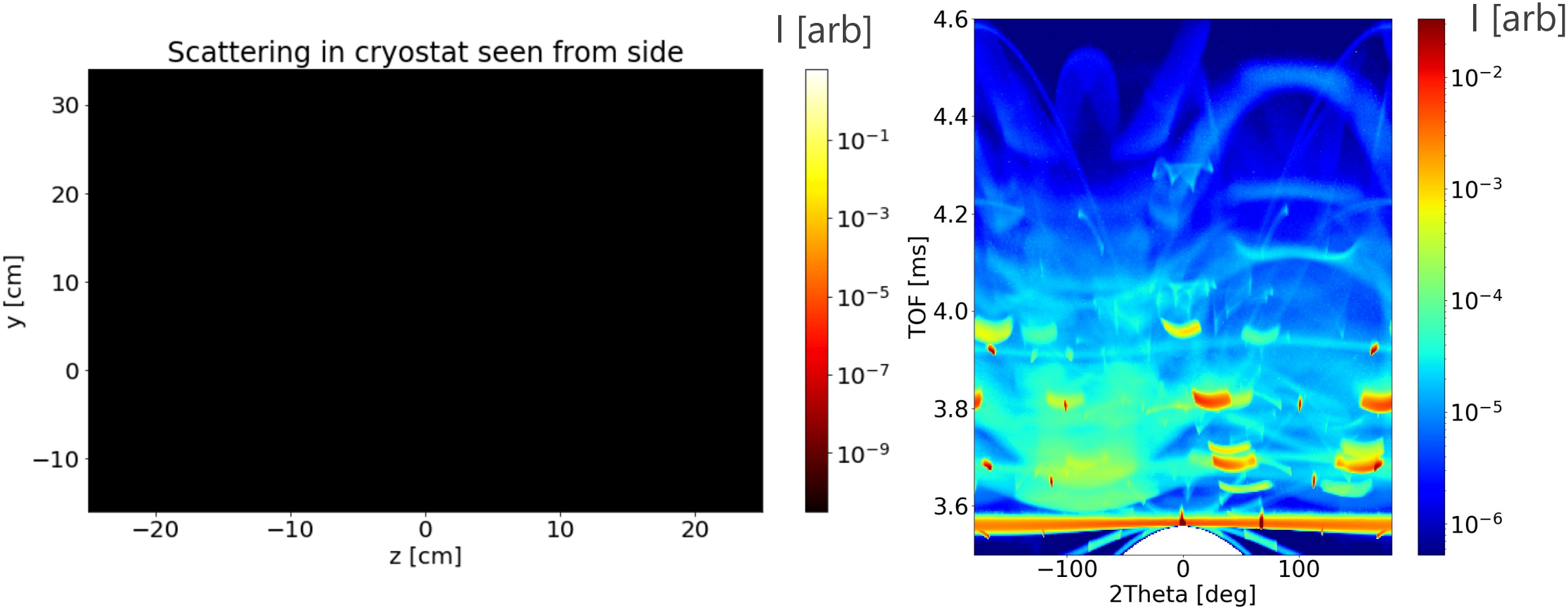
- Set of McStas components
- Works as a collection





Union components

Results

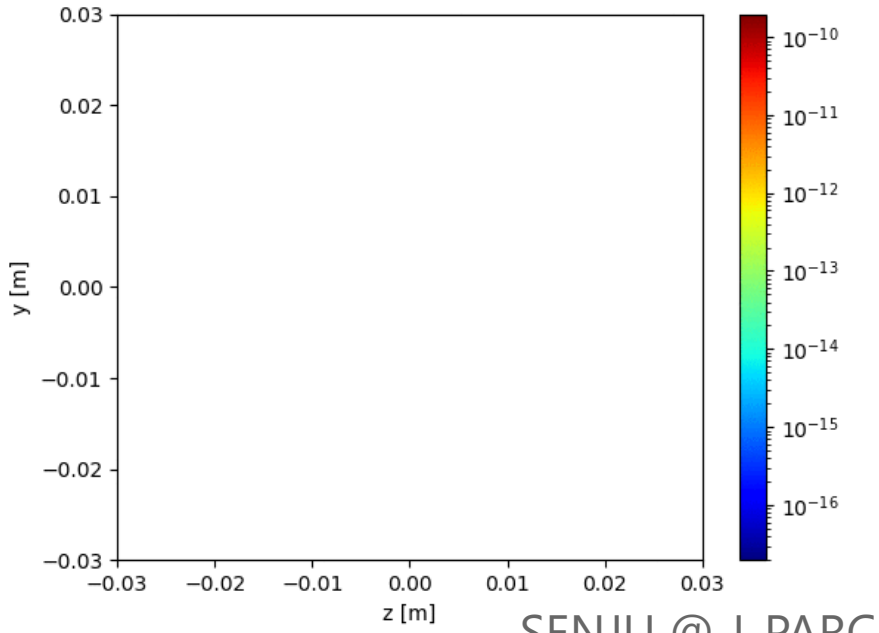


Union components

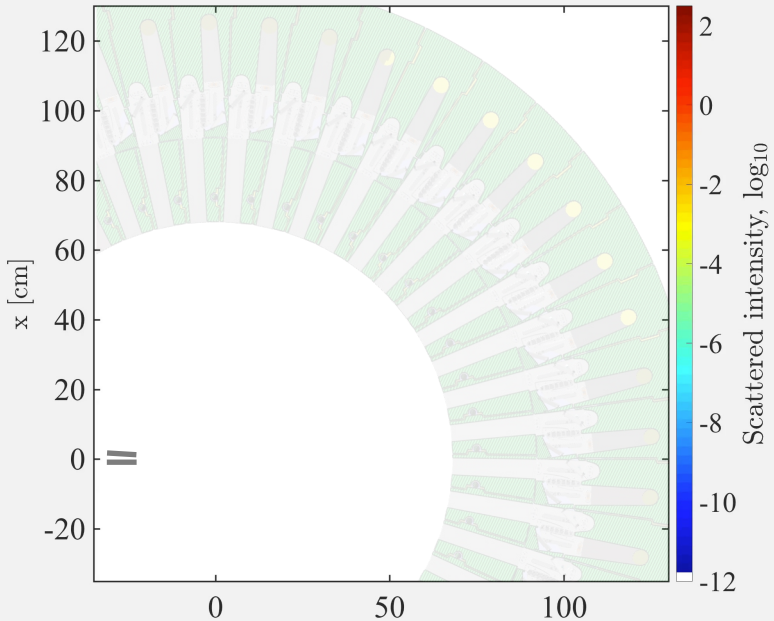
Instruments

- Joined beamtimes
- Simulated the instruments

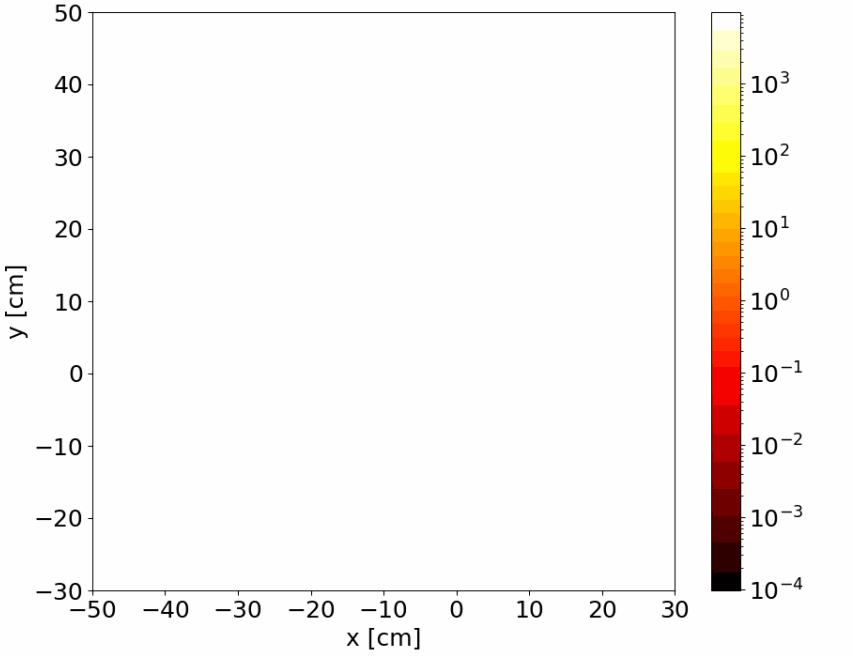
SNAP @ SNS



MACS @ NIST



SENJU @ J-PARC



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Software

guide_bot MATLAB

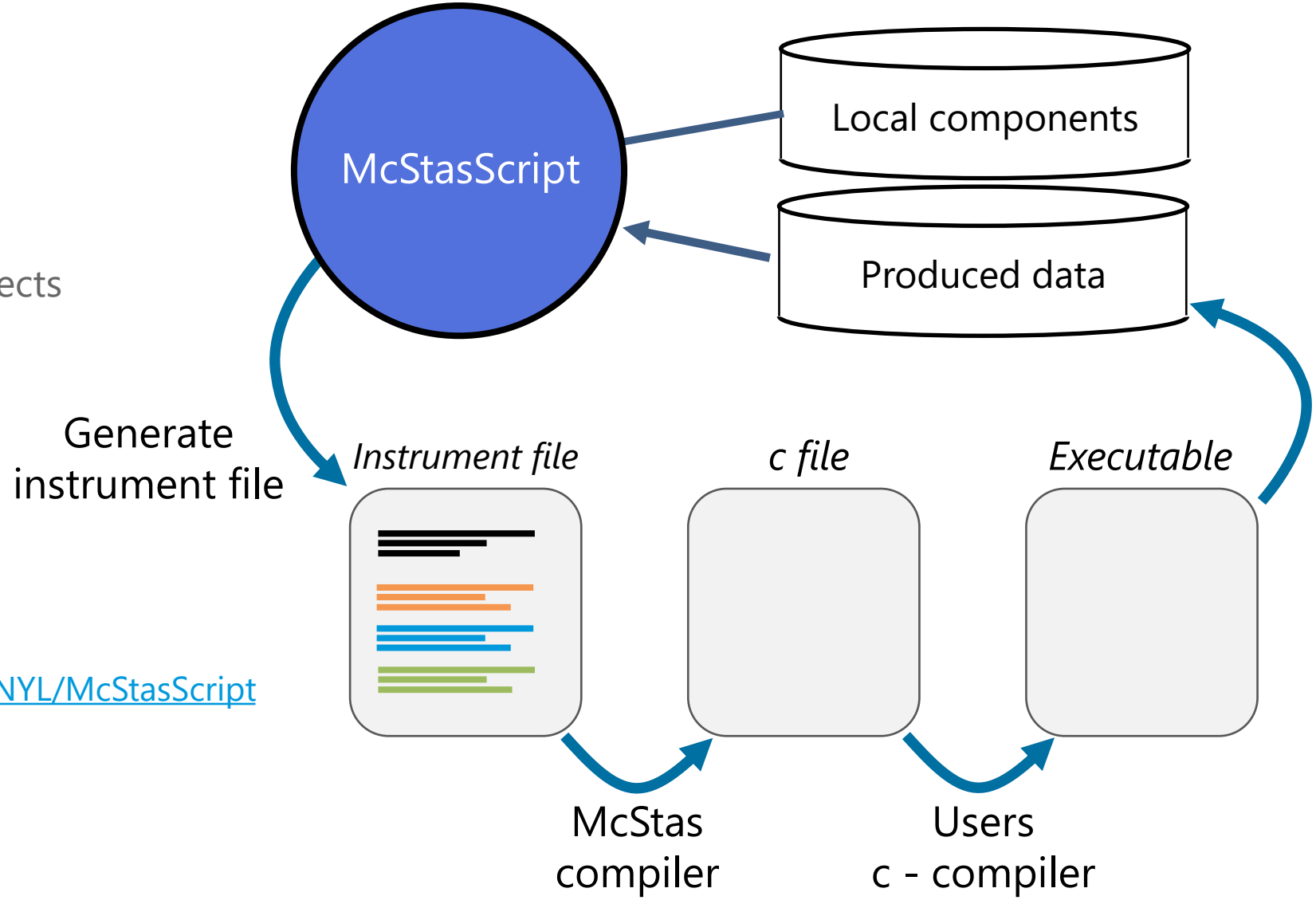
McStas Union components

McStasScript

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

```
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
```

- Autocompletion

```
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

```
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
```

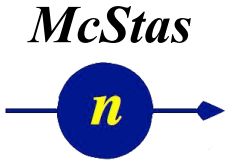
- Parameter overview

```
instrument.show_parameters()
```

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

McStasScript

Quick demo



- Set position
- For-loop
- Component list

```
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
```

```
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
```

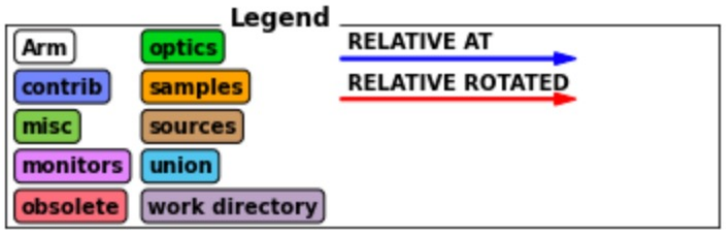
McStasScript

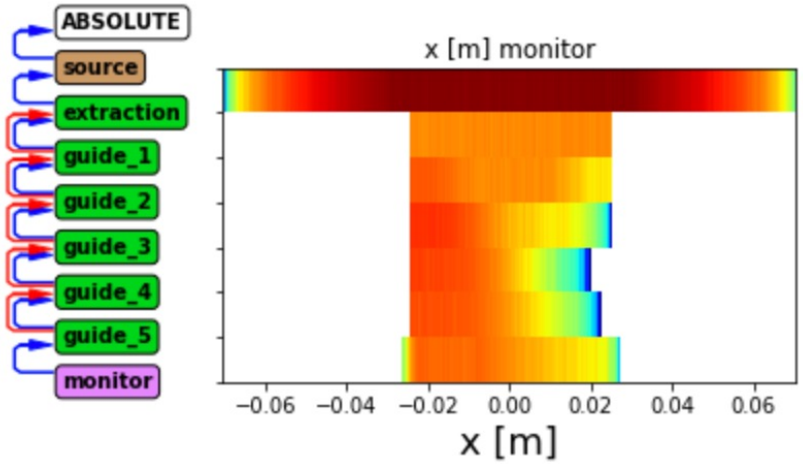
Quick demo

- Filename pitfall
- Diagrams

```
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

```
instrument.show_instrument()
```

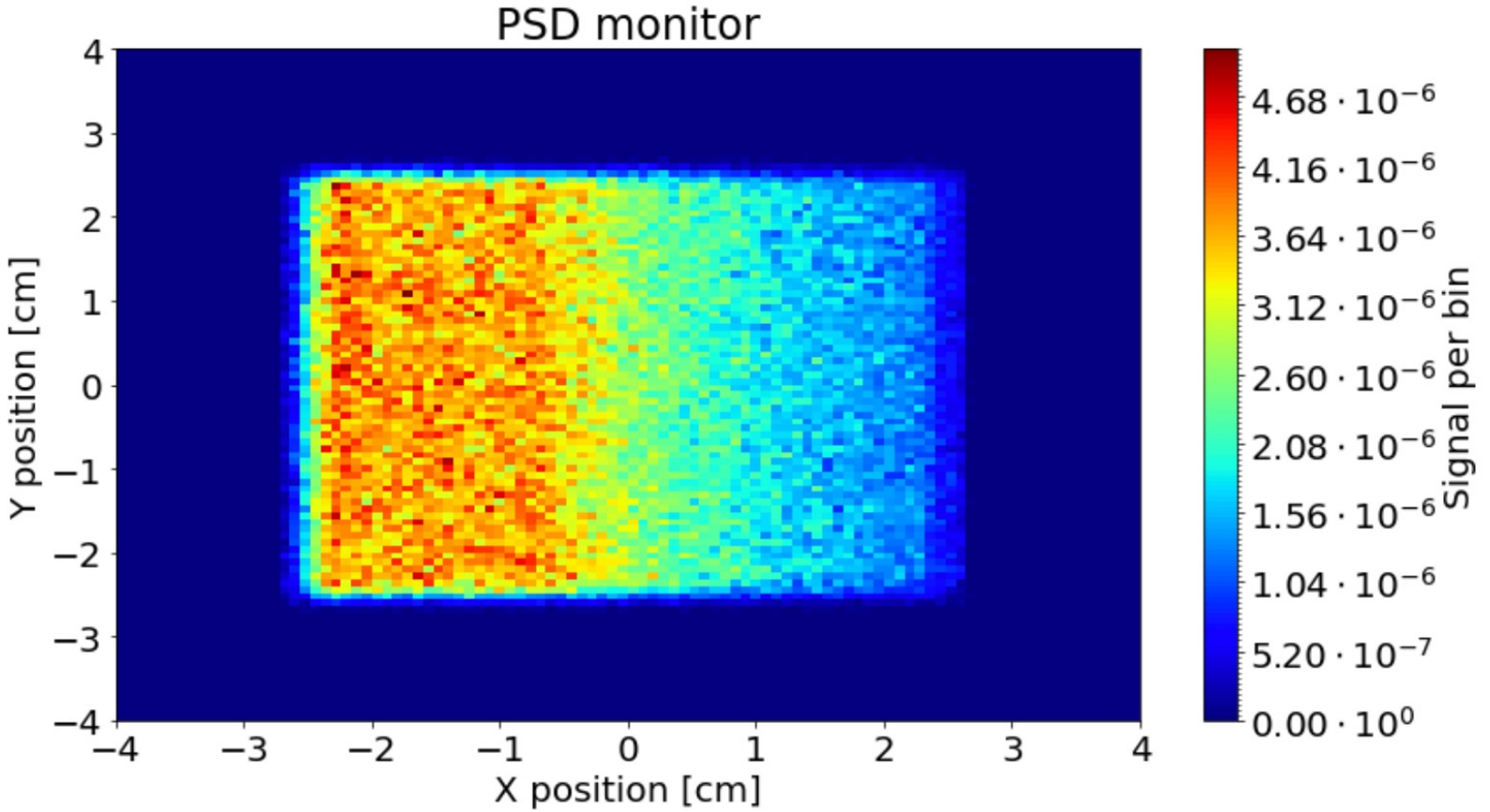
McStasScript

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
```

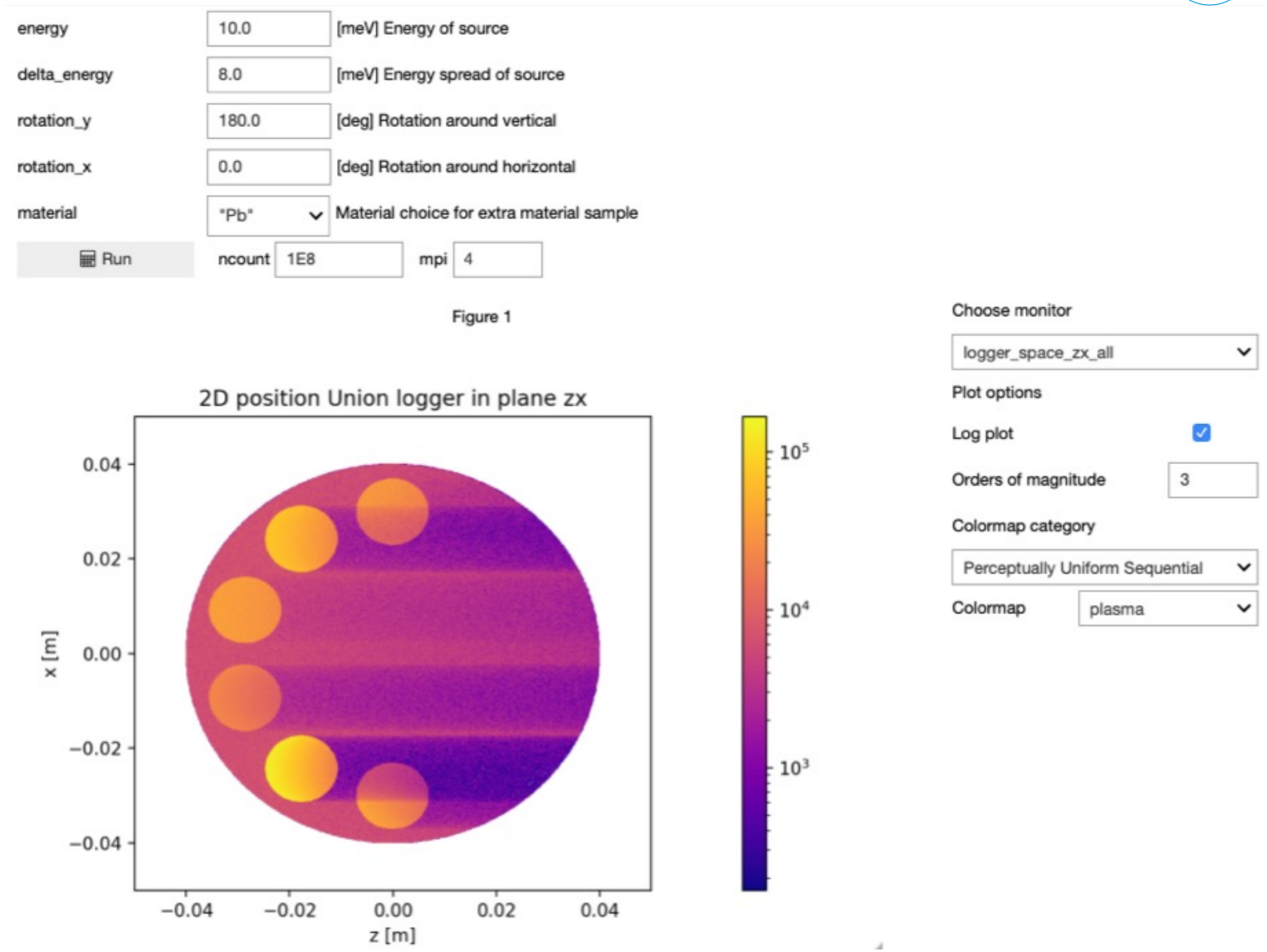
```
monitor.Intensity[20:28, 40:44]
```

```
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

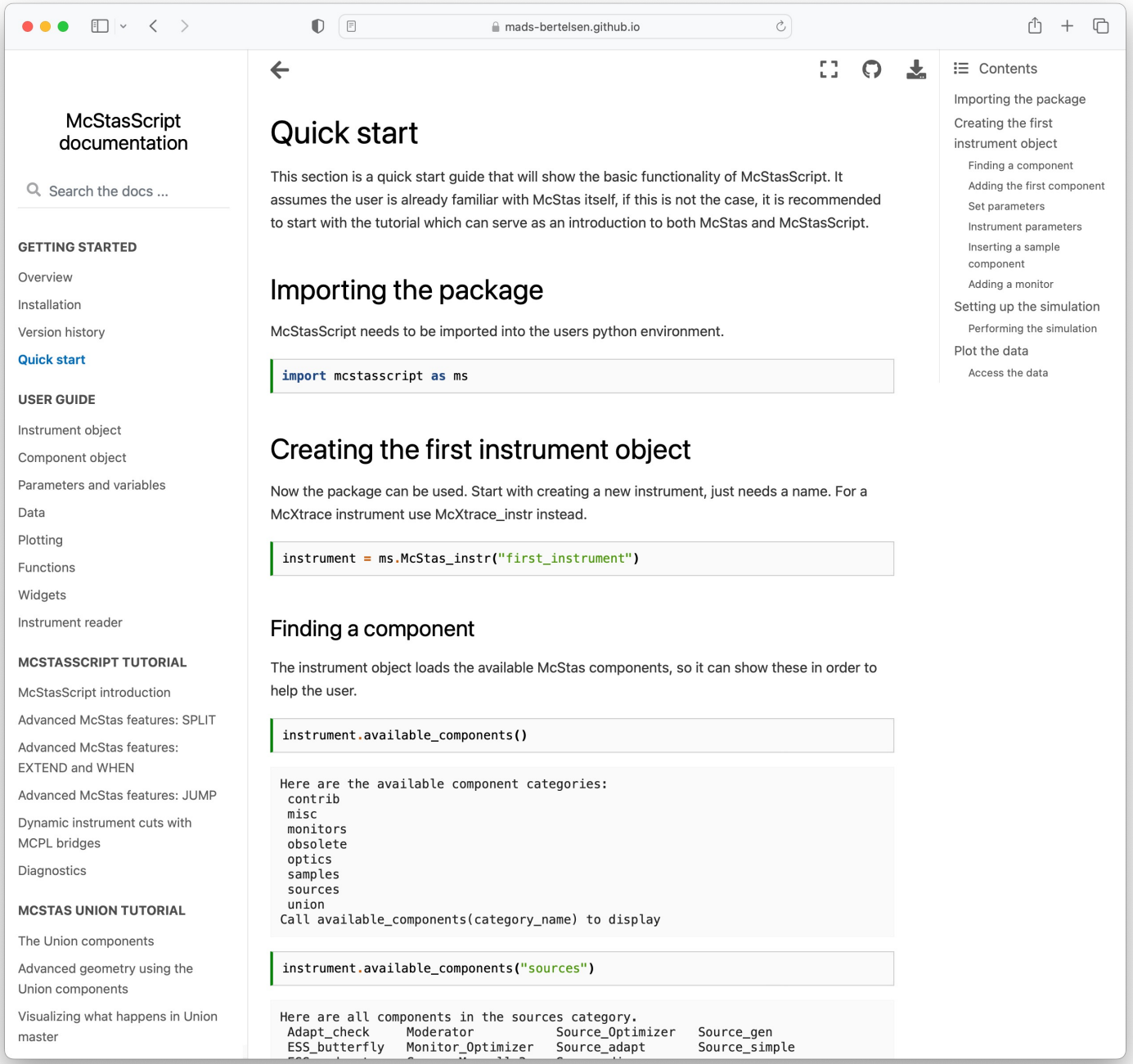


McStasScript

Documentation

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

- Workshop / School available



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Subject

Moderators | Neutron optics | Moderator - Optics coupling | Samples | Sample environments + Instrument backends

Software

guide_bot MATLAB

guide_bot Python

McStas Union components

McStasScript

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
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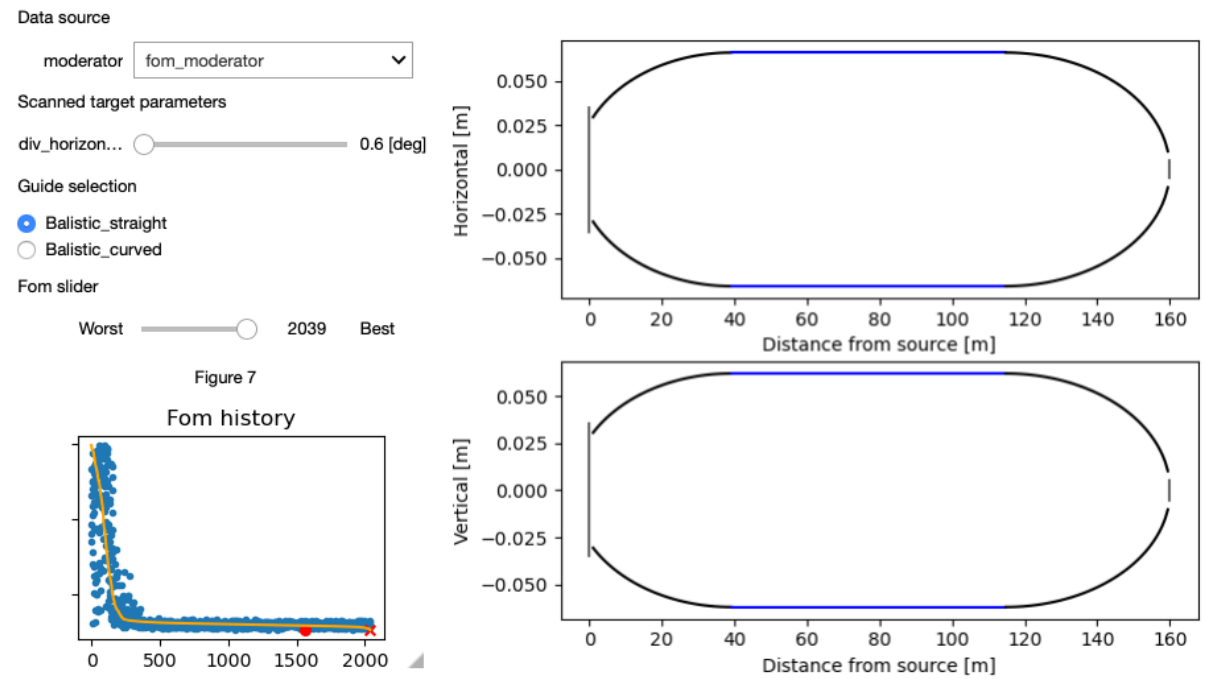
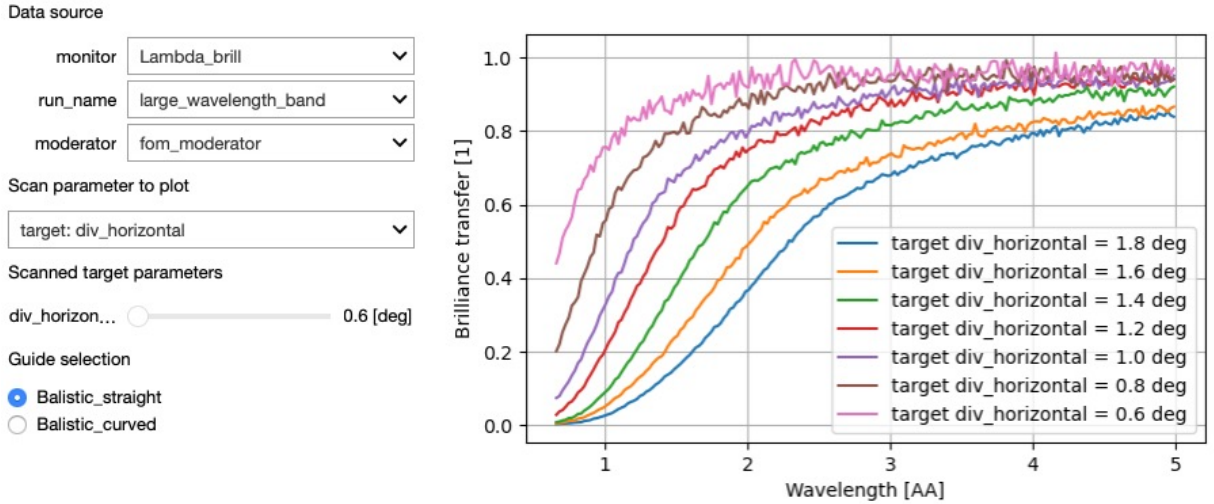
  - Use
- No license, more powerful
- Uses McStasScript
- Nice widgets for visualization





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Moderators	Neutron optics	Moderator - Optics coupling	Samples	Sample environments + Instrument backends	Detectors

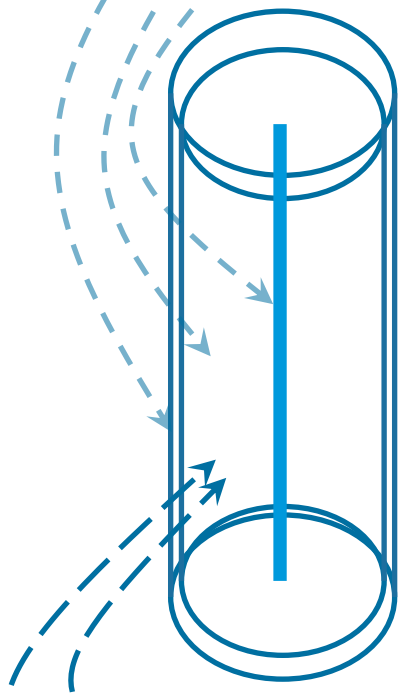
Software

guide_bot MATLAB	guide_bot Python
McStas Union components	
McStasScript	

Detectors

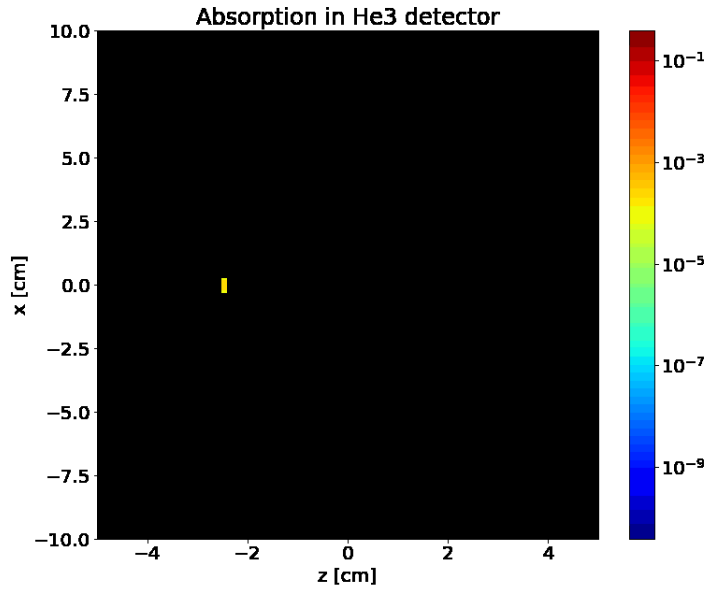
Overview

- Aluminium
- He3
- Wire

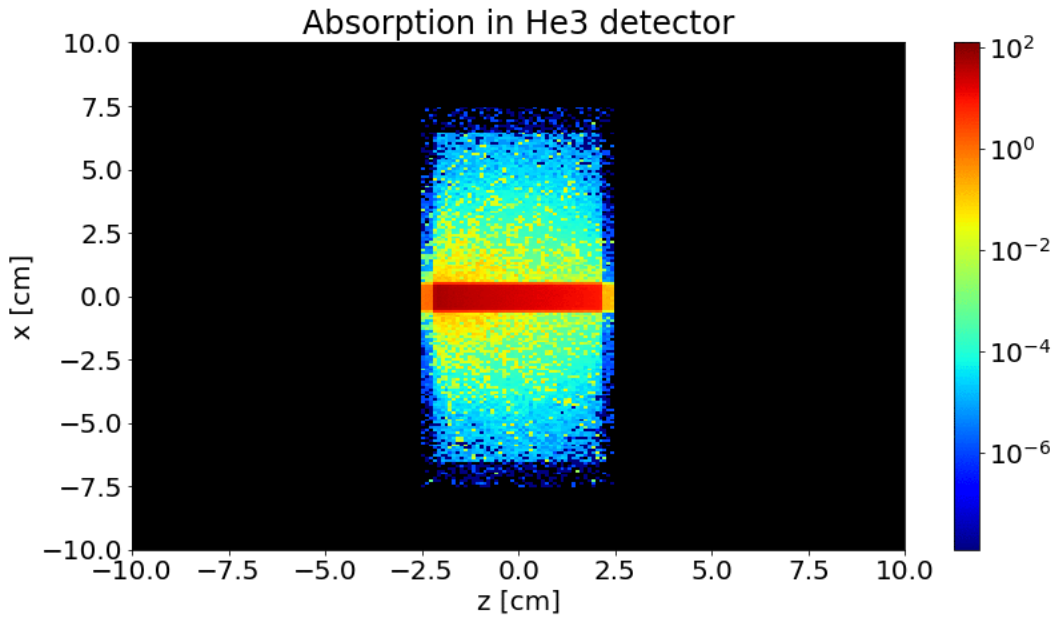


- Abs_logger_1D_space_tof
- Abs_logger_event

Small wavelength interval



Large wavelength interval



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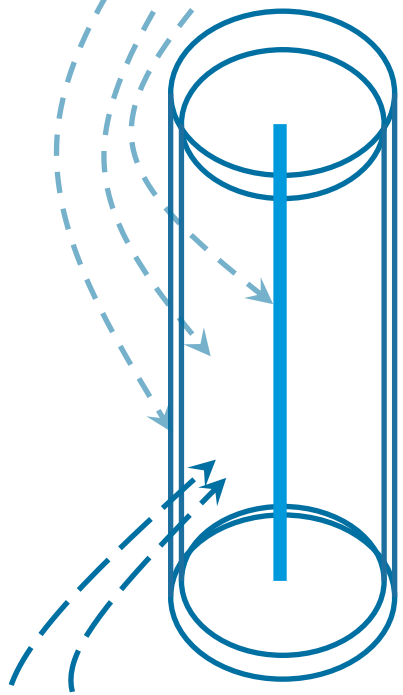

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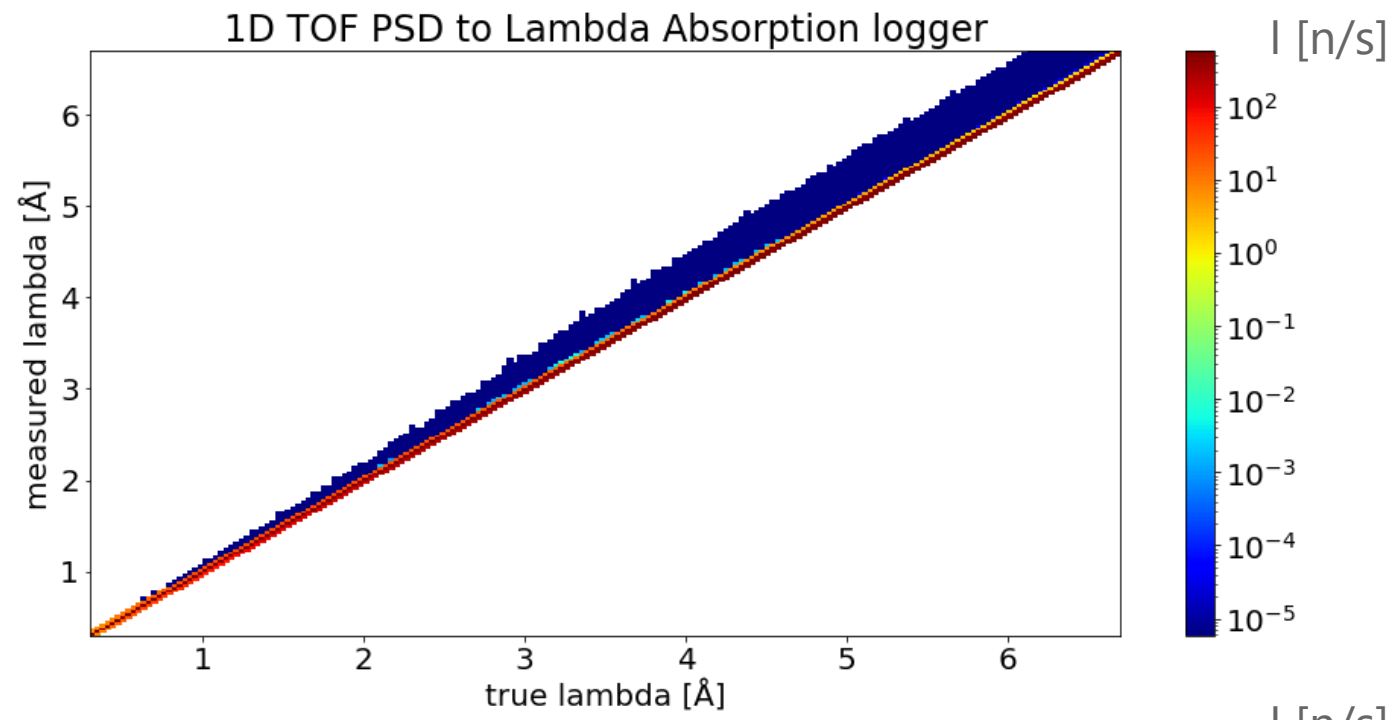
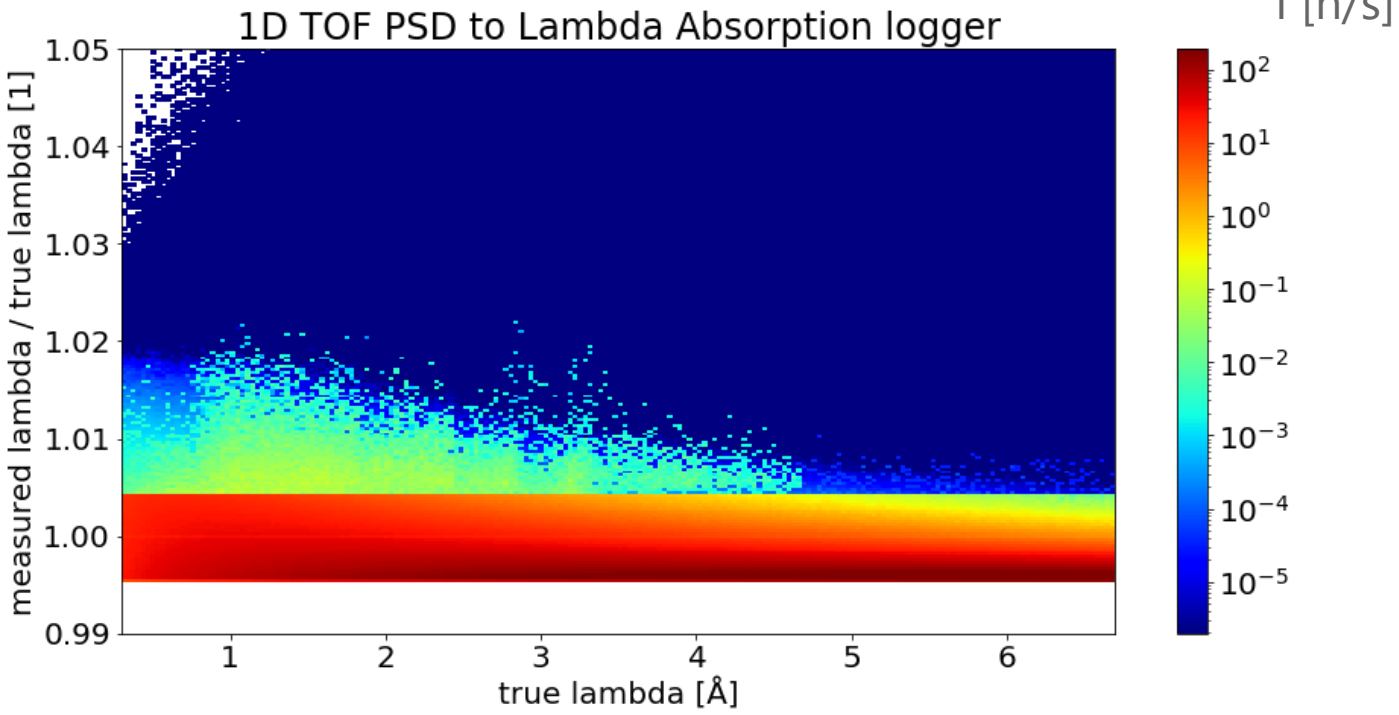
- Abs_logger_event





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

MIRROTRON

Timeline

Overview

University of Copenhagen - Kim Lefmann

European Spallation Source

My work with McStas

Position

elor	Master	PhD 4+4	Scientific Assistant	PhD 4+4	Post Doc	Post Doc	Perm

Subject

Moderators	Neutron optics	Moderator - Optics coupling	Samples	Sample environments + Instrument backends	Detectors

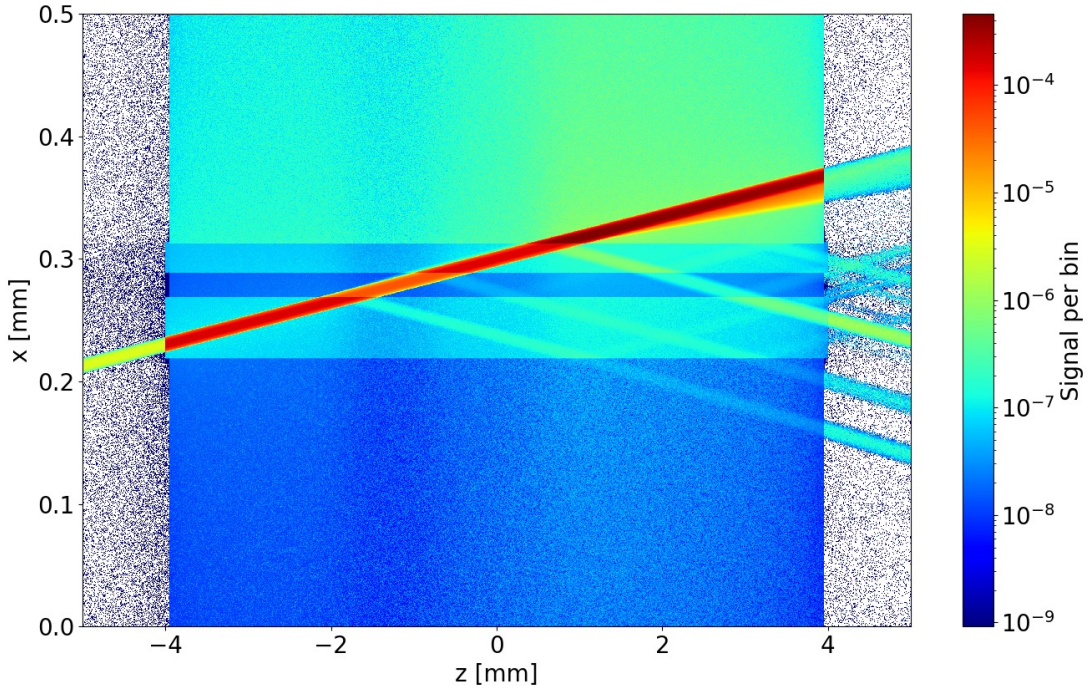
Software

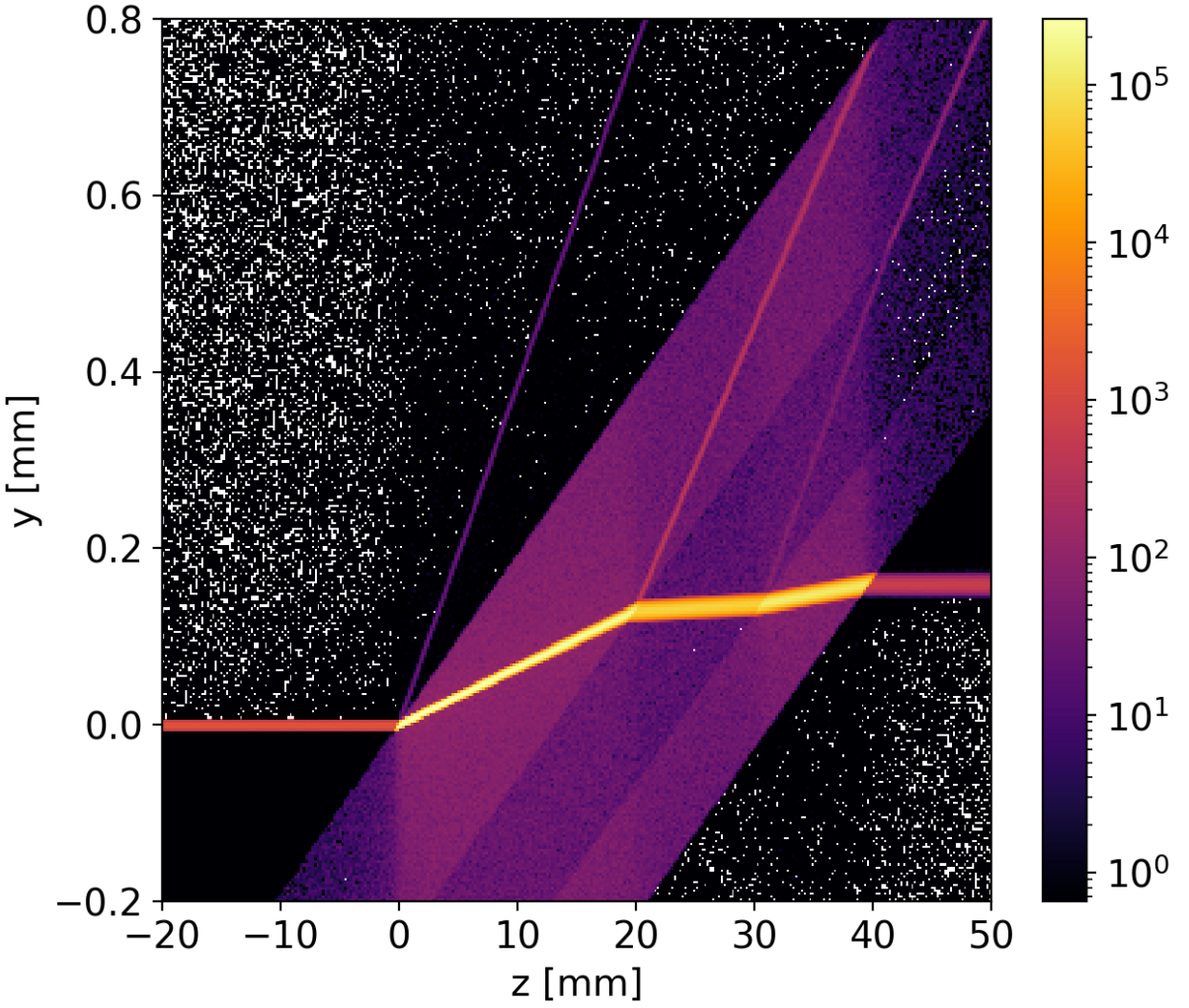
guide_bot MATLAB	guide_bot Python
McStas Union components	
McStasScript	

Outlook

Union features

- Refraction in Union components
- Surface effects in general

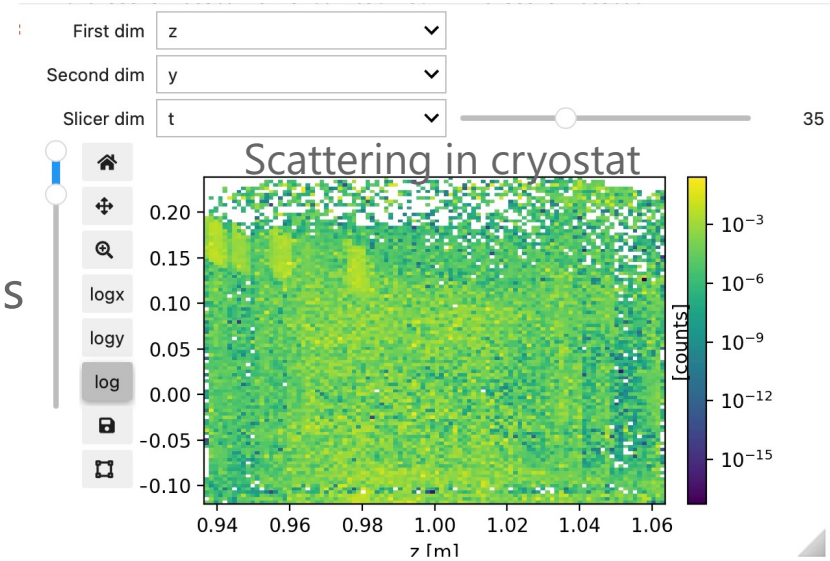


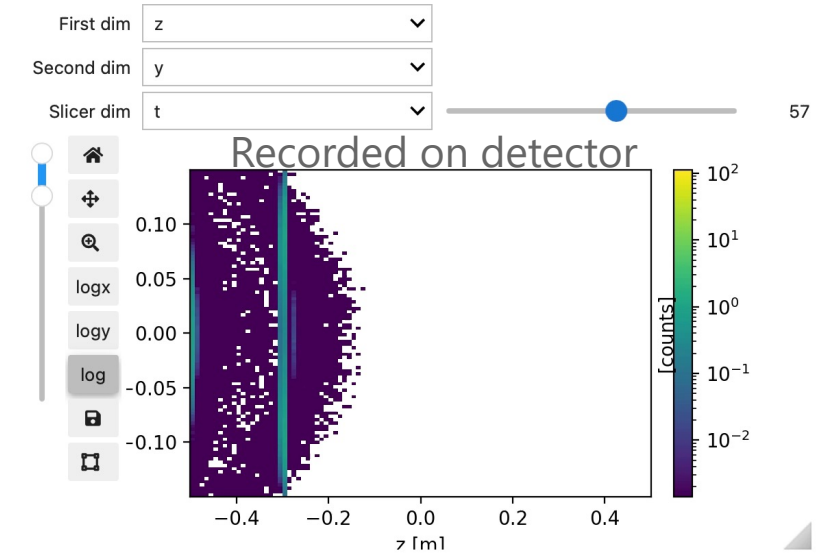


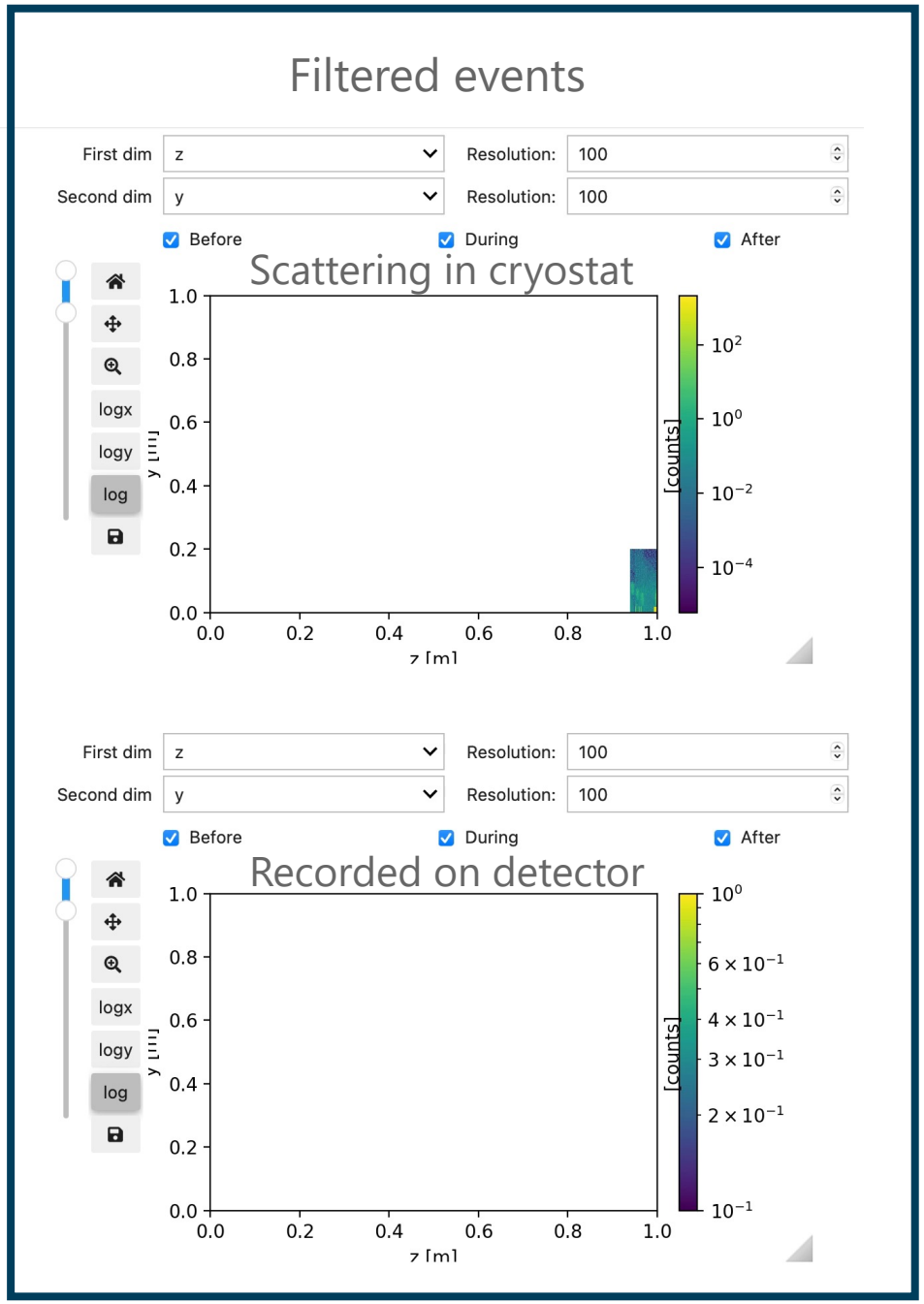
Outlook

Widget

- Event data widget
- Explore ray histories







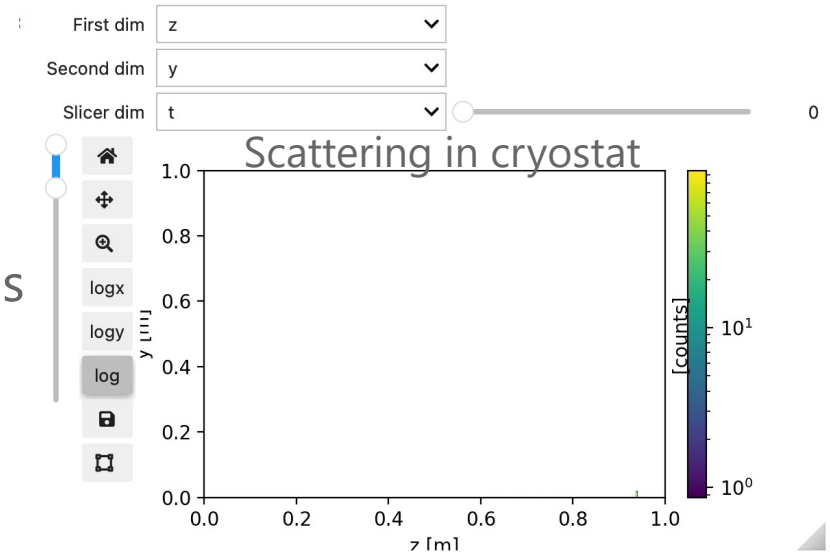
scipp

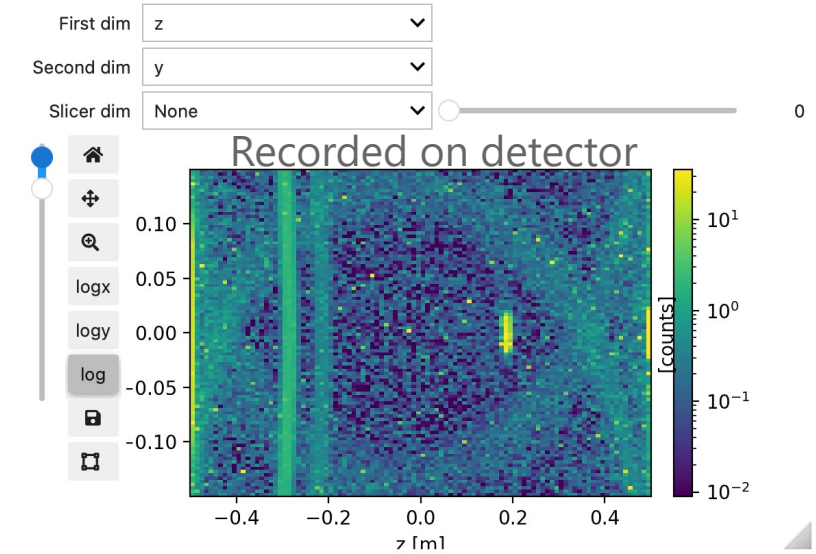
plopp

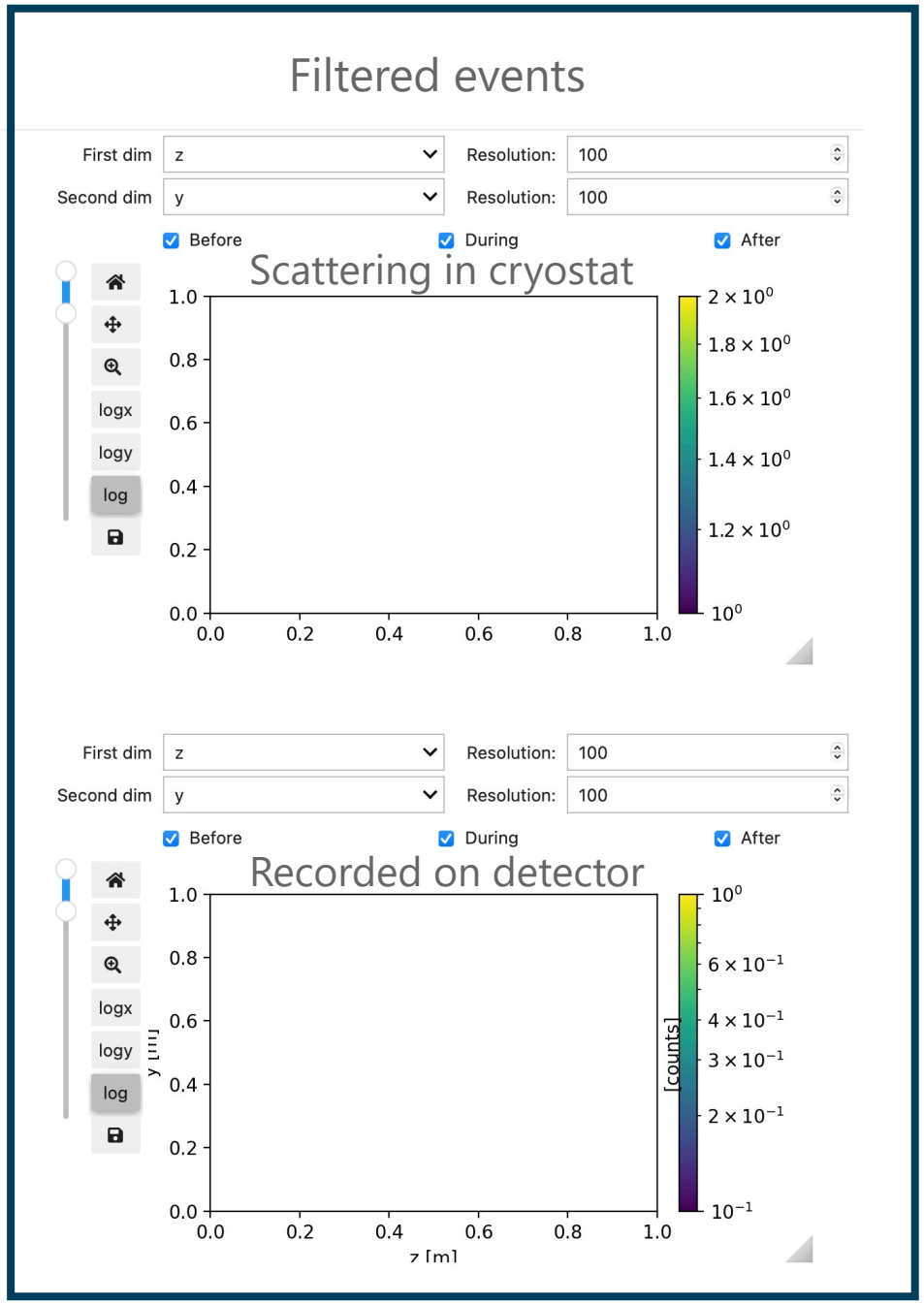
Outlook

Widget

- Event data widget
- Explore ray histories







scipp

plopp

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

2023-10-10