ORNL McStas course 2018
- McStas Union components

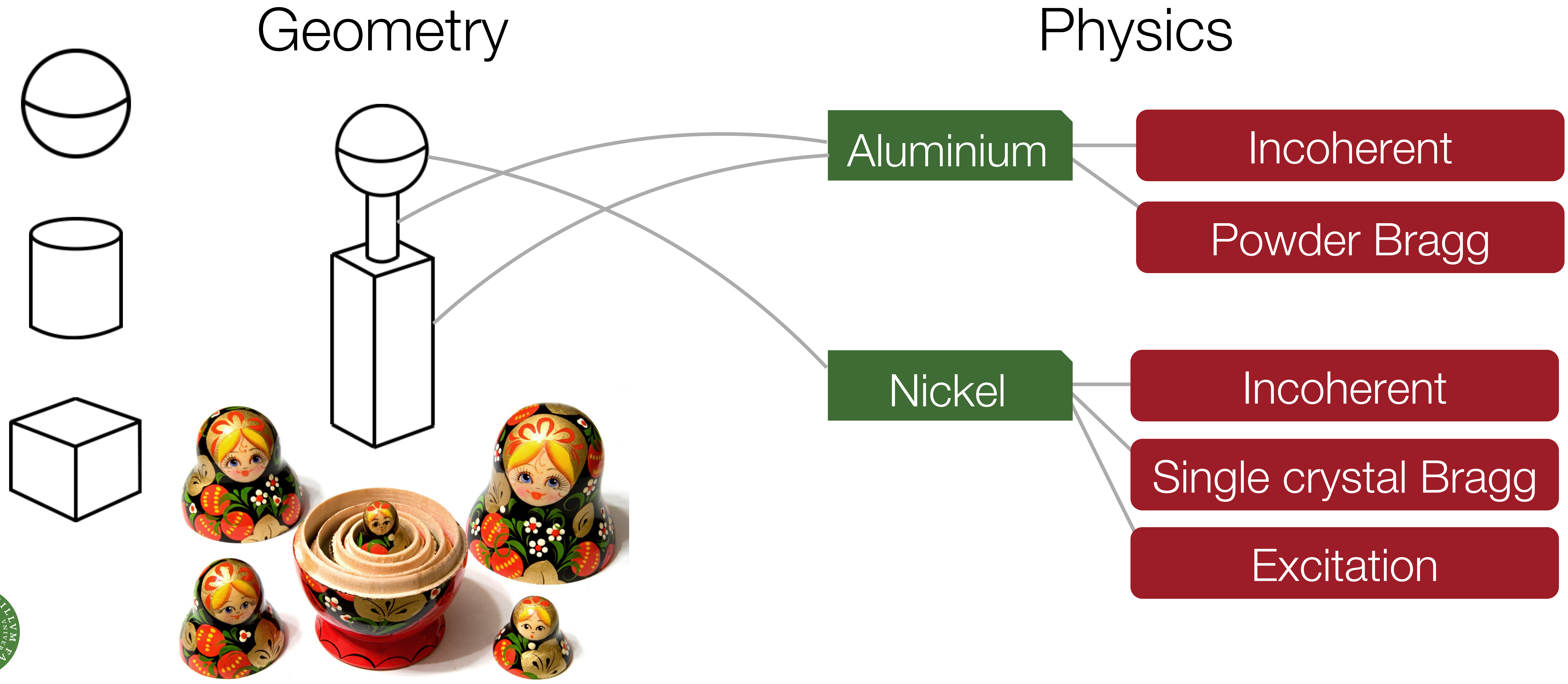
- Slides from Mads Bertelsen
University of Copenhagen

Background in McStas

- Sample holders with complicated geometry
- Many different materials
- Inside sample environment
- Co aligned crystals
- Twinned crystals

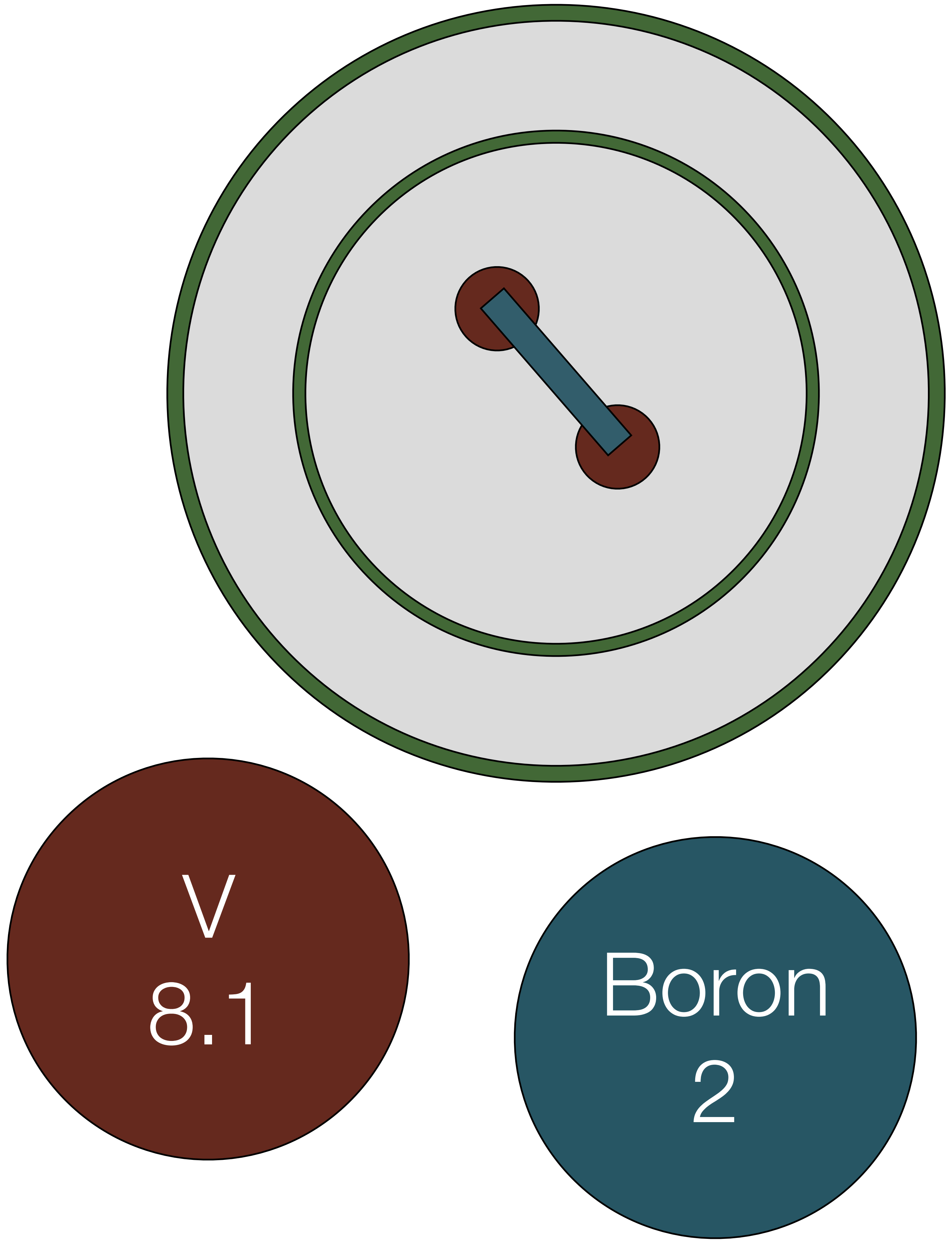
Photo by Pia Ray Jensen

McStas Union components - Idea



McStas Union components - Priority

- Each geometry is assigned a material definition and a priority
- Priority decides which material is simulated in regions where several overlap
- This can be used to construct complex geometries with a range of materials



McStas Union components - Use

```
COMPONENT Al_incoherent = Incoherent_process(
  sigma=4*0.0082,packing_factor=1,
  unit_cell_volume=66.4)
AT (0,0,0) ABSOLUTE

COMPONENT Al_powder = Powder_process(
  reflections="Al.laz")
AT (0,0,0) ABSOLUTE

COMPONENT Al = Union_make_material(
  my_absorption=100*4*0.231/66.4,
  process_string=“Al_incoherent,Al_powder”)
AT (0,0,0) ABSOLUTE
```

sigma in [barns]
unit_cell_volume in [Å^3]

my [1/m] = cross section per unit cell / unit cell volume

McStas Union components - Use

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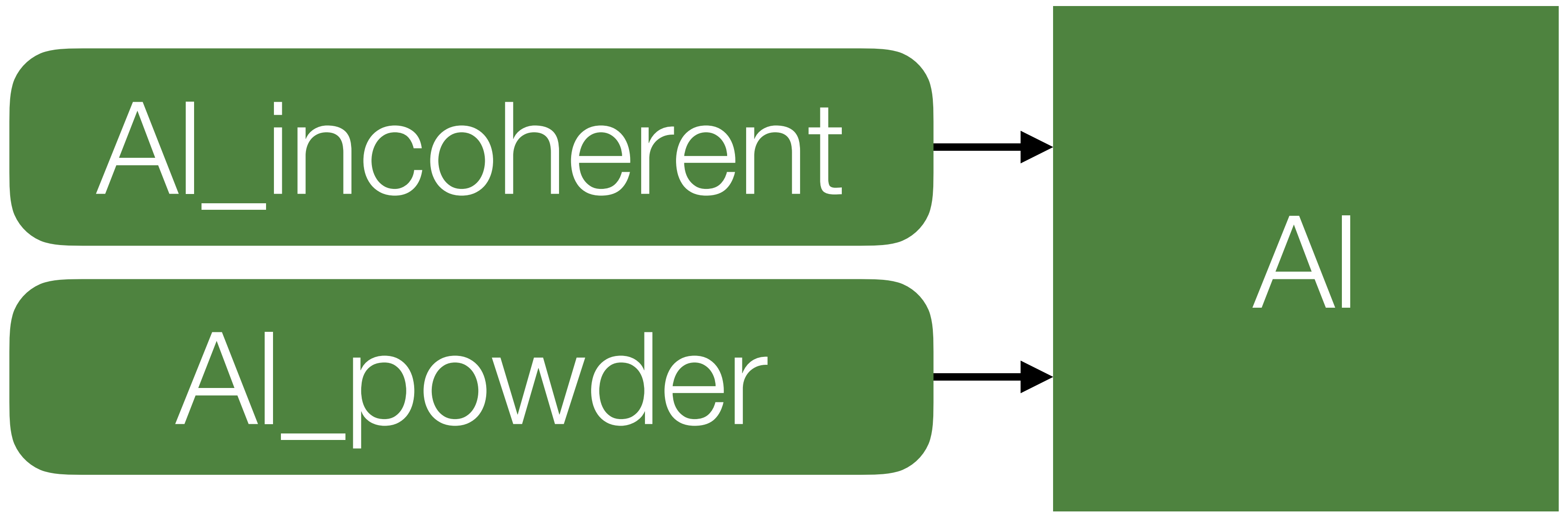
sigma in [barns]

unit_cell_volume in [$Å^3$]



my [1/m] = cross section per unit cell / unit cell volume

McStas Union components - Use

```
COMPONENT cryostat_shell = Union_cylinder(
  radius_input=0.15,height_input=0.4,
  priority_input=10,material_string="Al")
AT (0,0.0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target
```

Uses our Al definition!

```
COMPONENT cryostat_vacuum = Union_cylinder(
  radius_input=0.147,height_input=0.4,
  priority_input=11,material_string="Vacuum")
AT (0,0.0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target
```

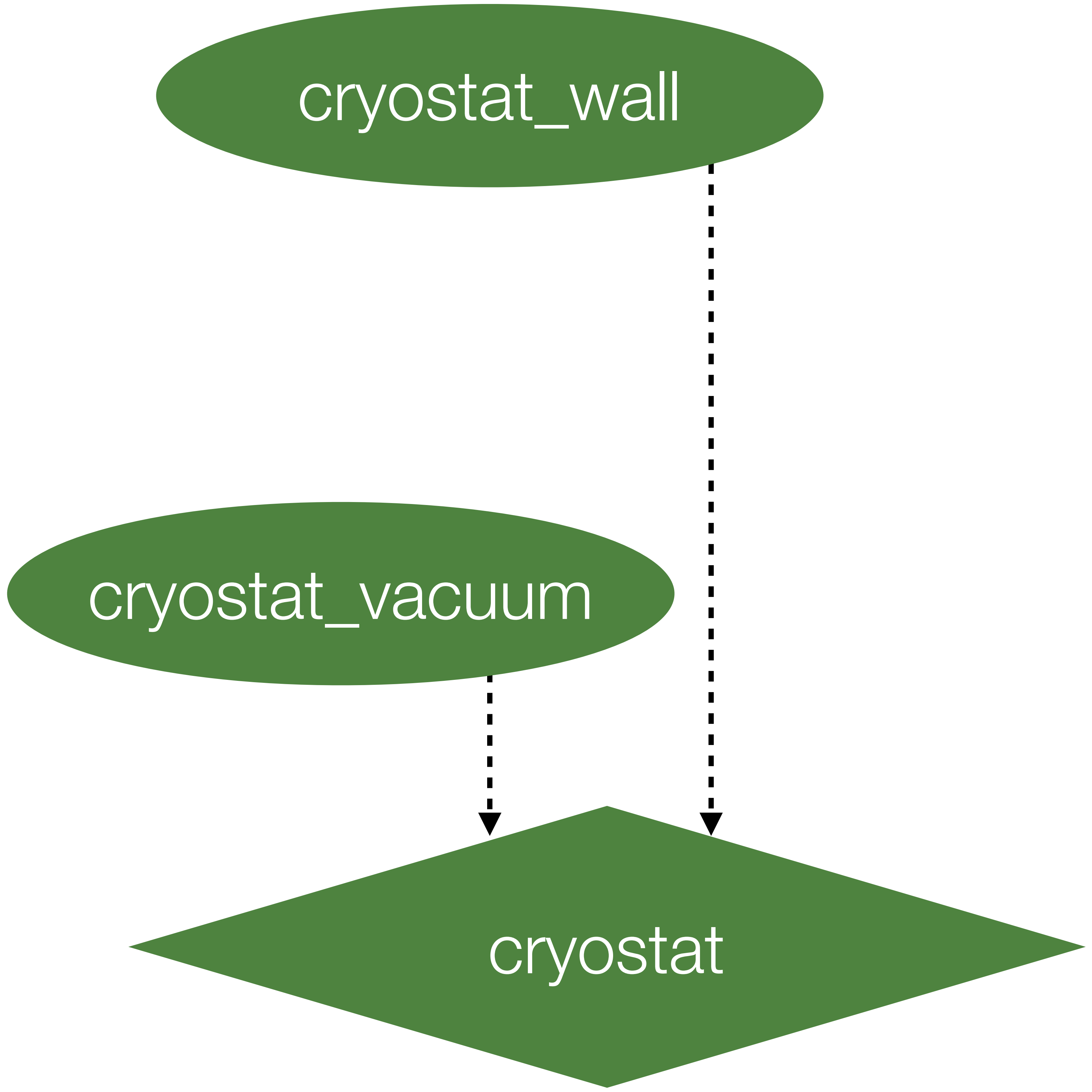
Uses default material definition

Does not do any simulation what so ever

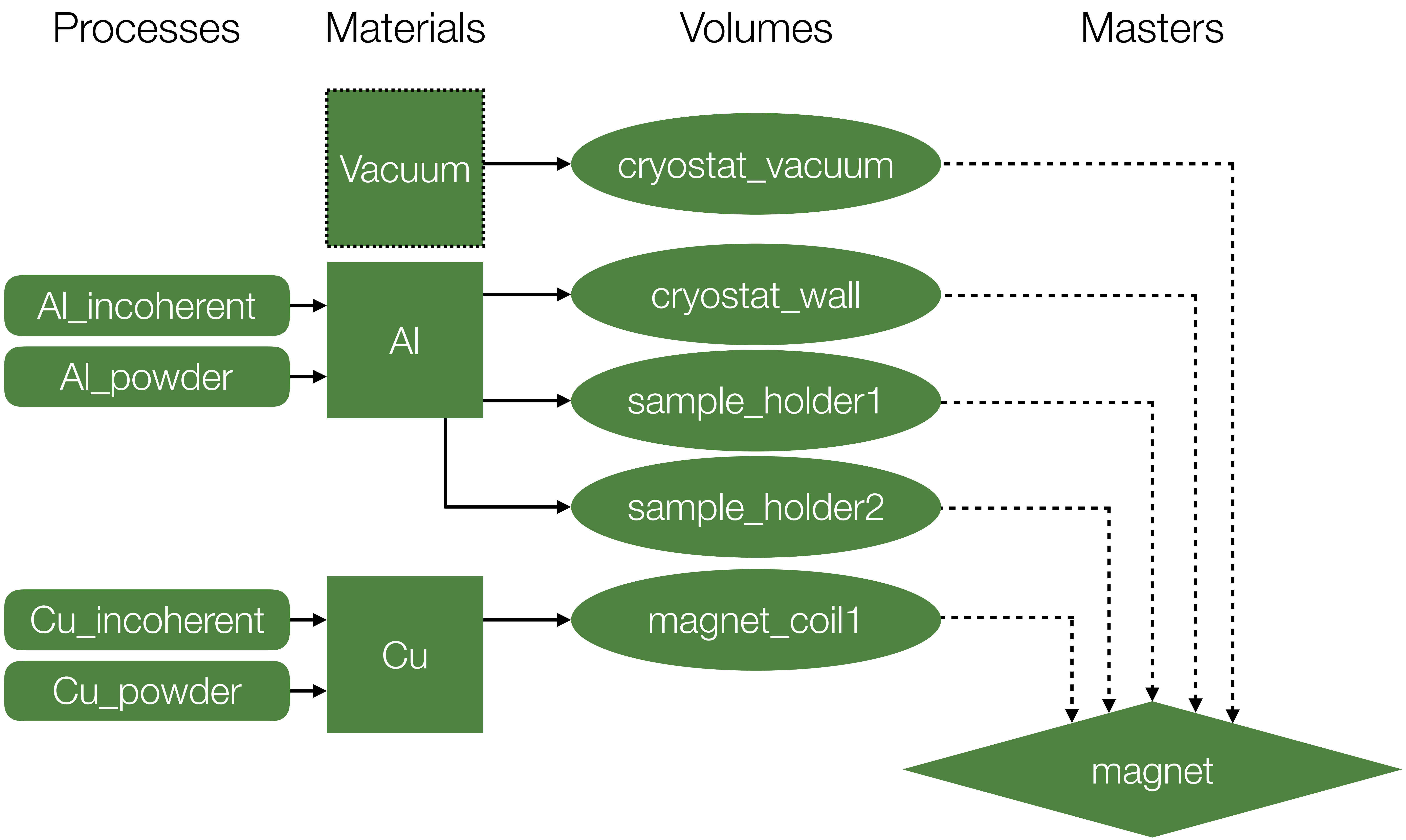
McStas Union components - Use

```
COMPONENT cryostat_shell = Union_cylinder(
  radius_input=0.15,height_input=0.4,
  priority_input=10,material_string="Al")
AT (0,0.0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target

COMPONENT cryostat_vacuum = Union_cylinder(
  radius_input=0.147,height_input=0.4,
  priority_input=11,material_string="Vacuum")
AT (0,0.0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target

COMPONENT cryostat = Union_master()
AT (0,0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target
```

The Union_master does the simulation

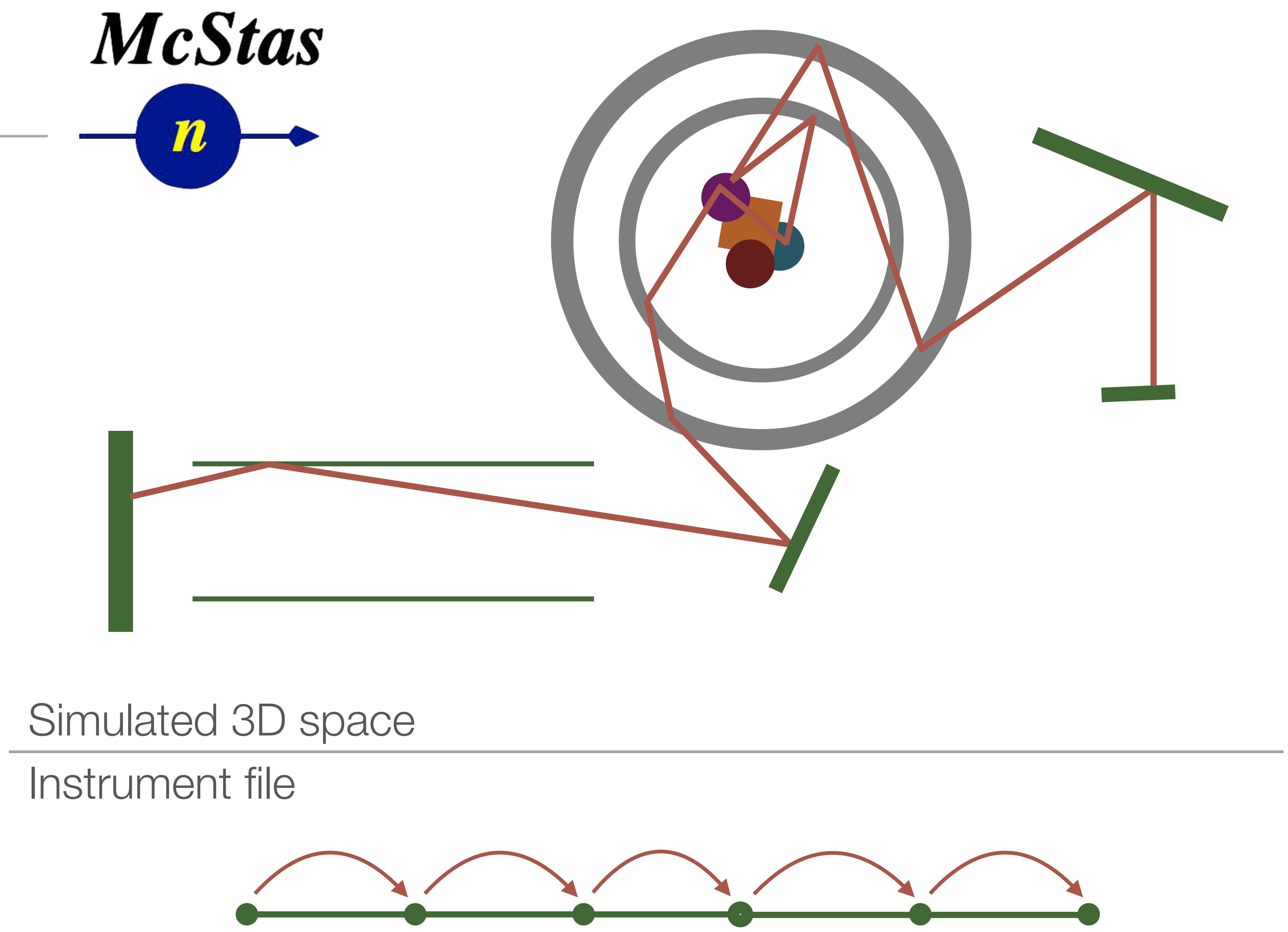


McStas Union components - Use



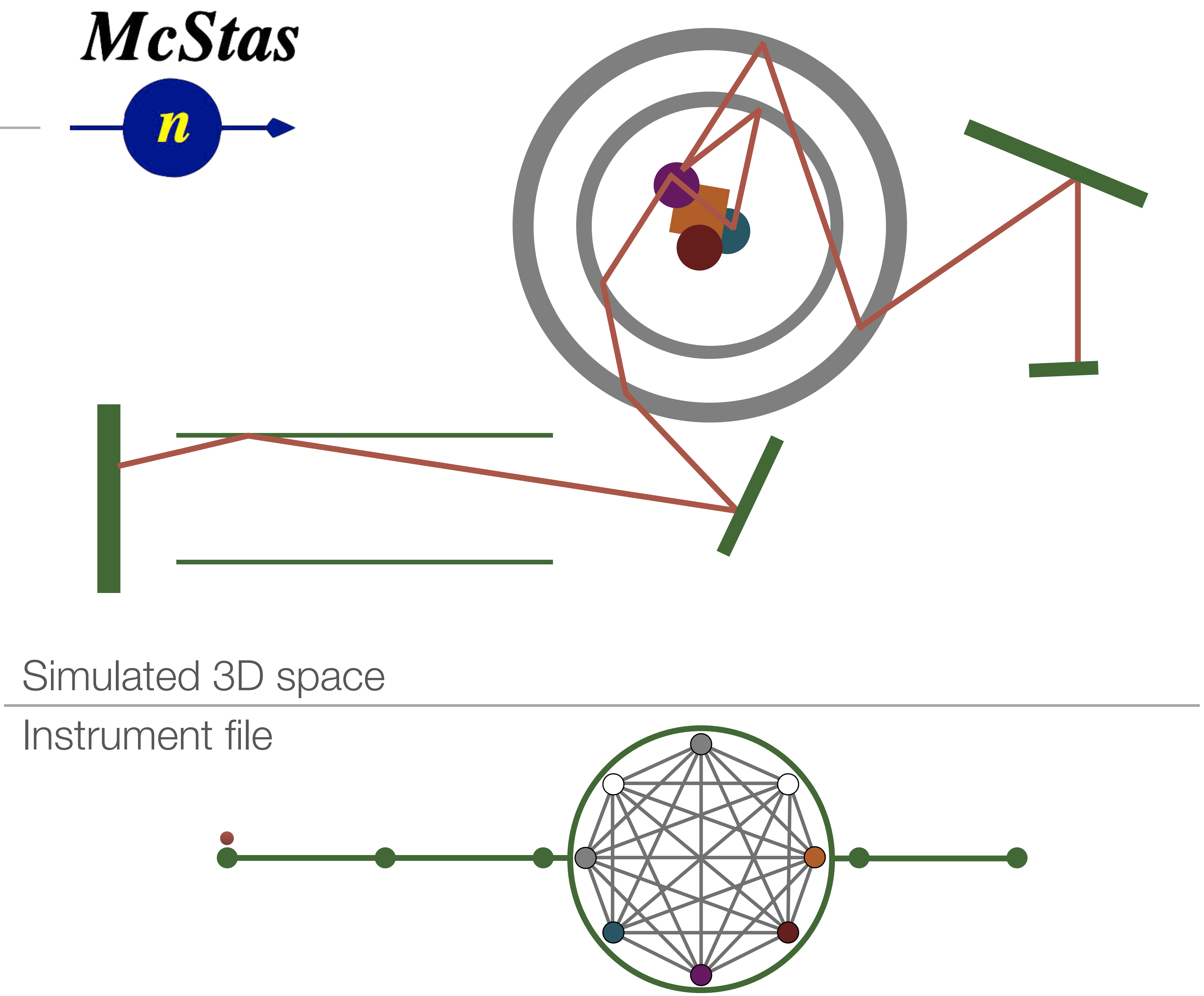
Union in instrument file

- Only the Union_master component affects the McStas simulation



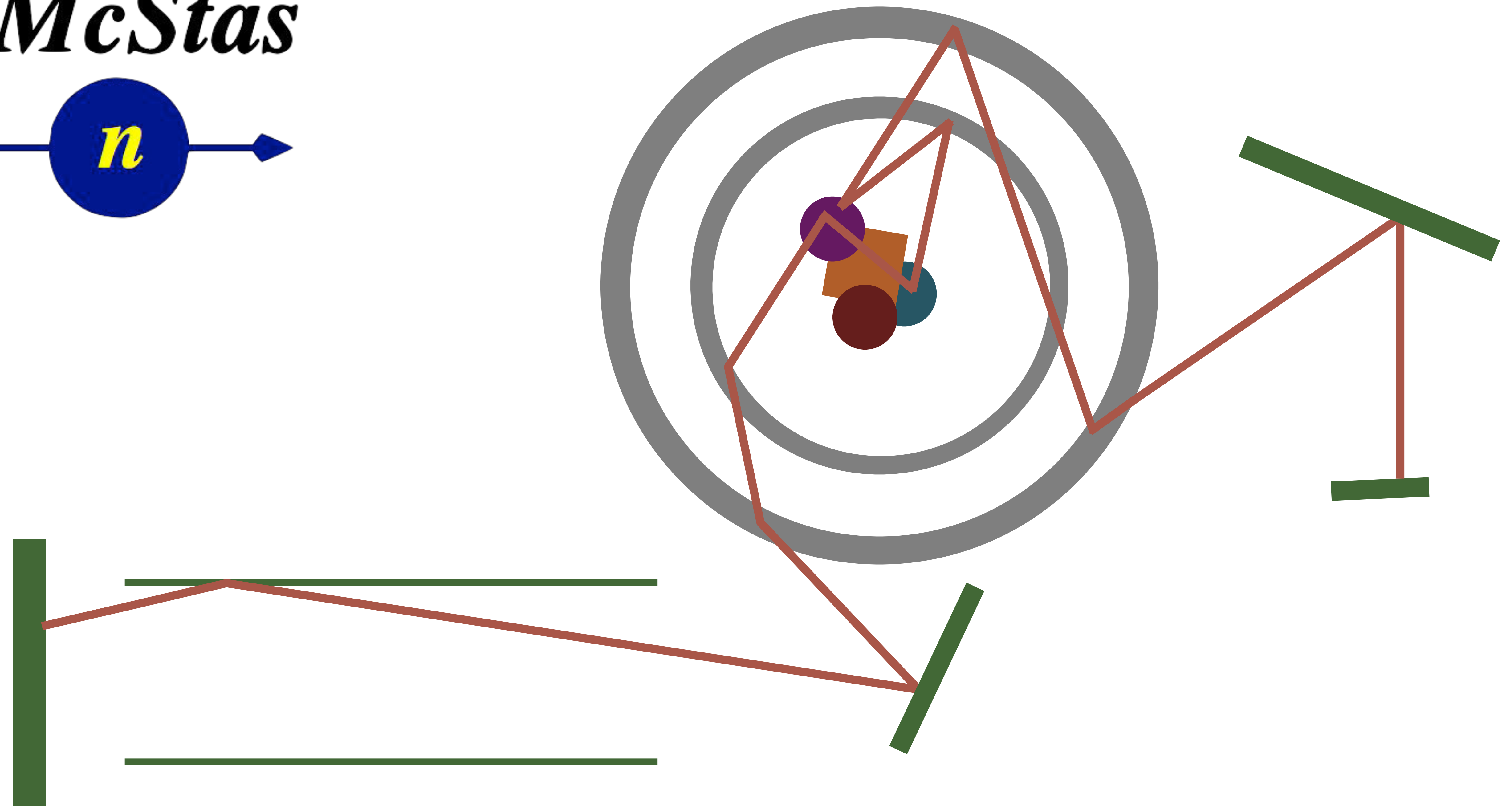
Union in instrument file

- Only the Union_master component affects the McStas simulation
- The Union_master component uses a network for propagation



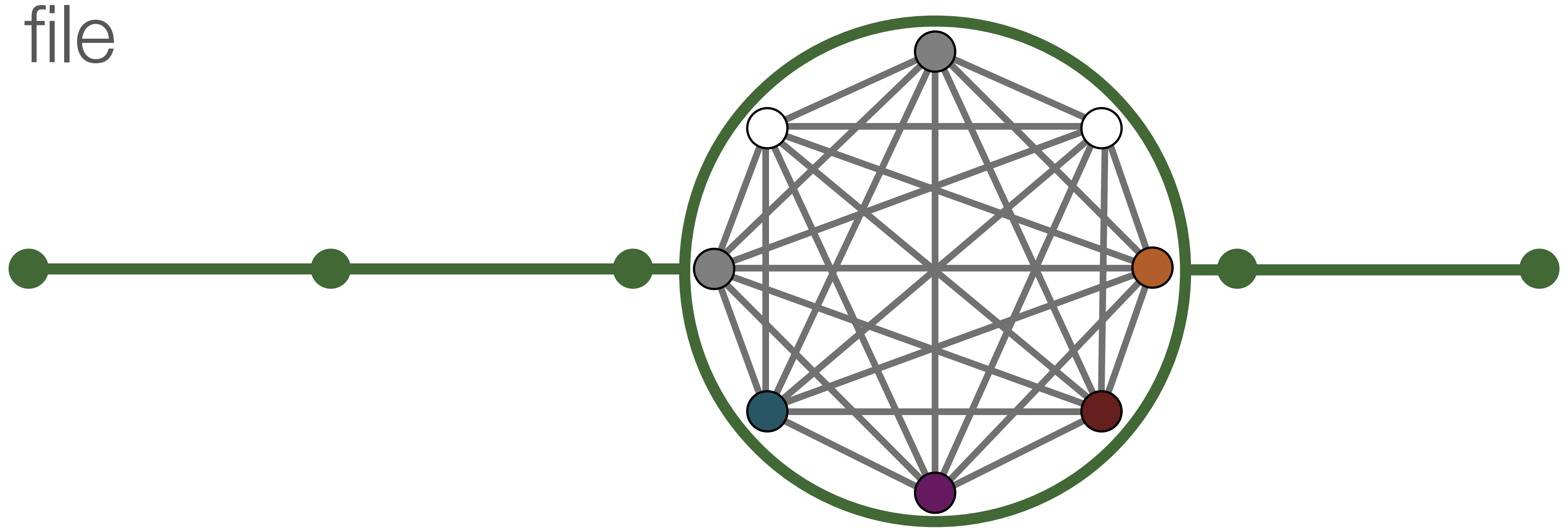
Union in instrument file

- Only the Union_master component affects the McStas simulation
- The Union_master component uses a network for propagation
- Analysis prior to simulation reduces the network complexity



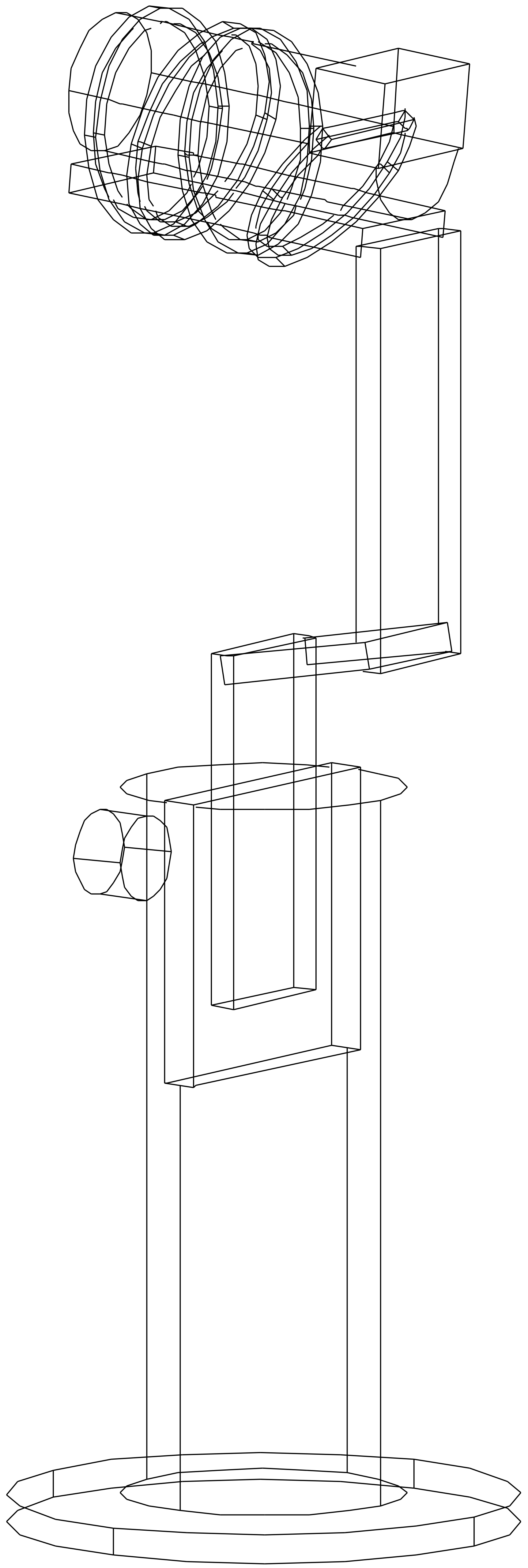
Simulated 3D space

Instrument file



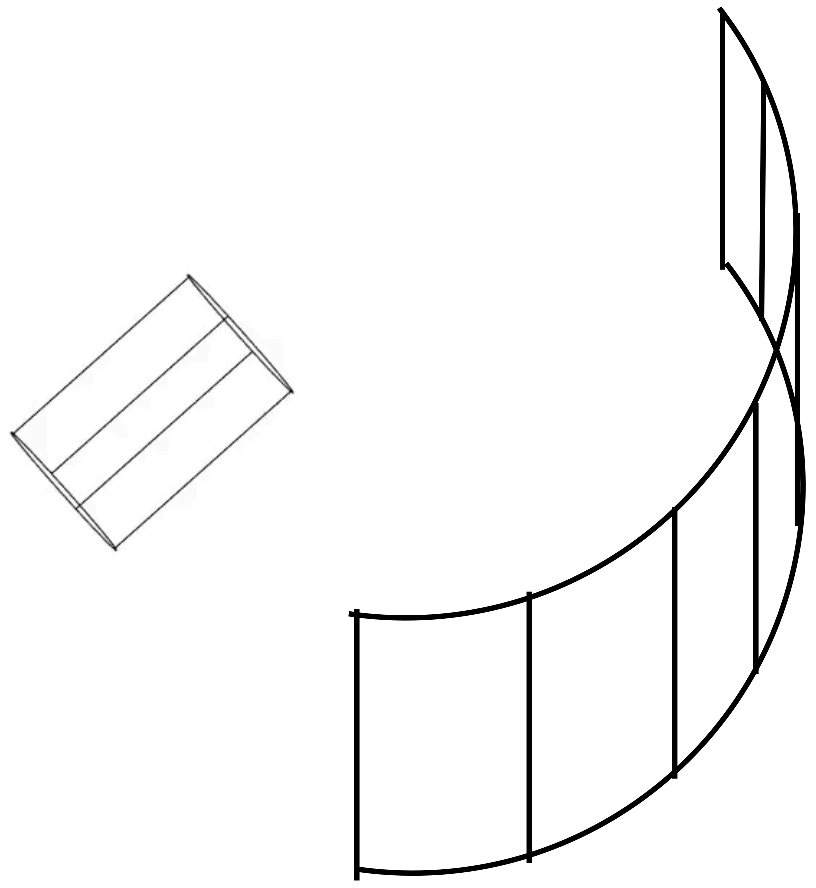
McStas Union components

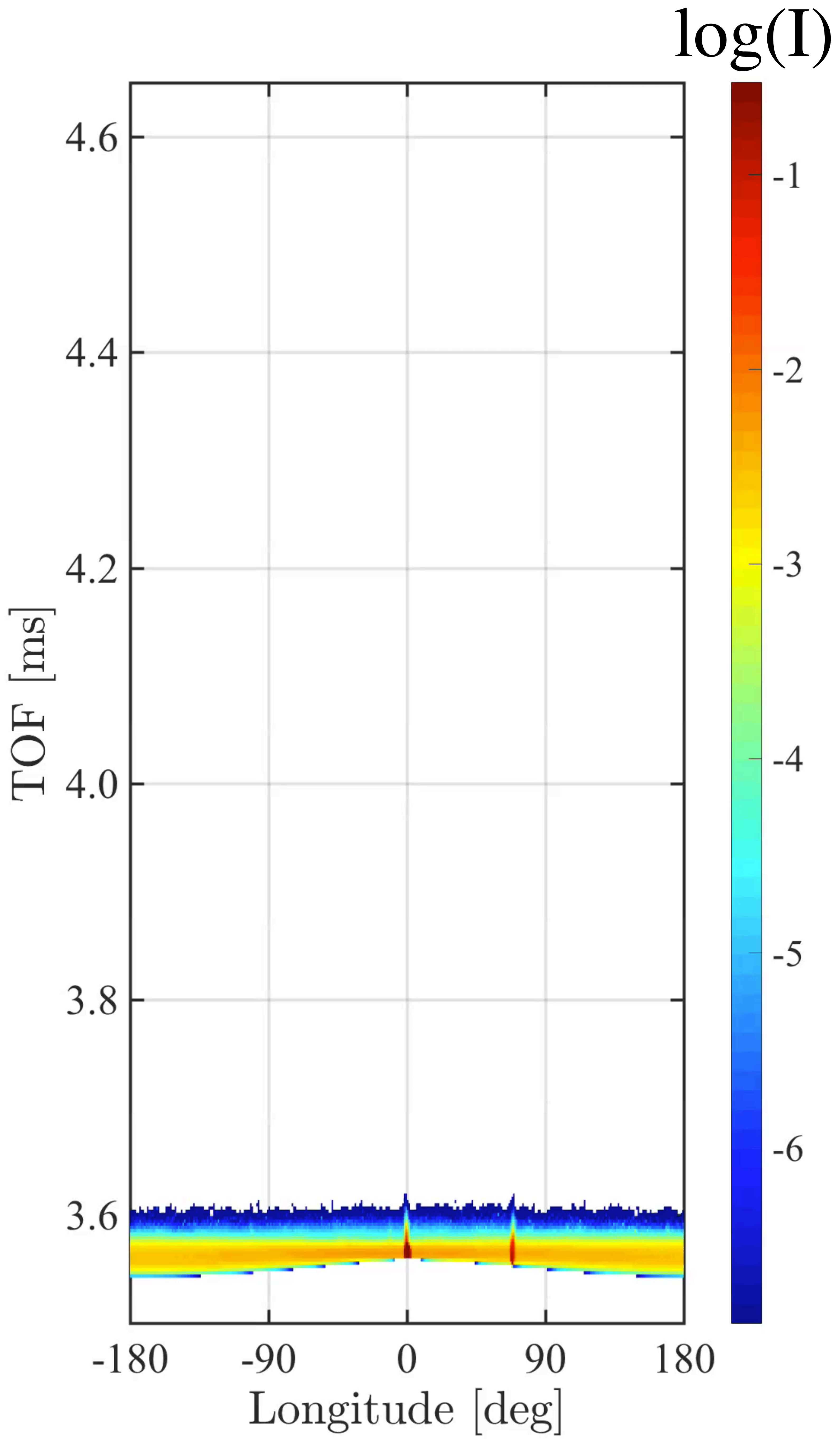
- Replicated from picture
- Easily assembled using Union components in McStas
- Material definitions made for sample / Aluminium
- Al absorption exaggerated



Building a sample

5 meV beam





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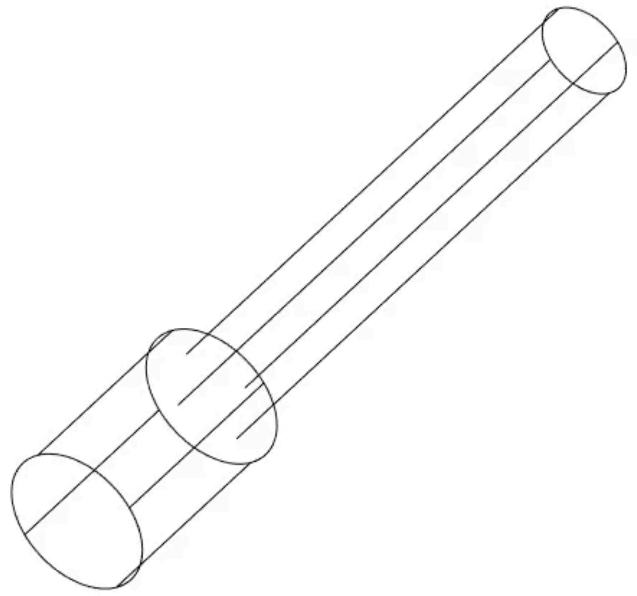

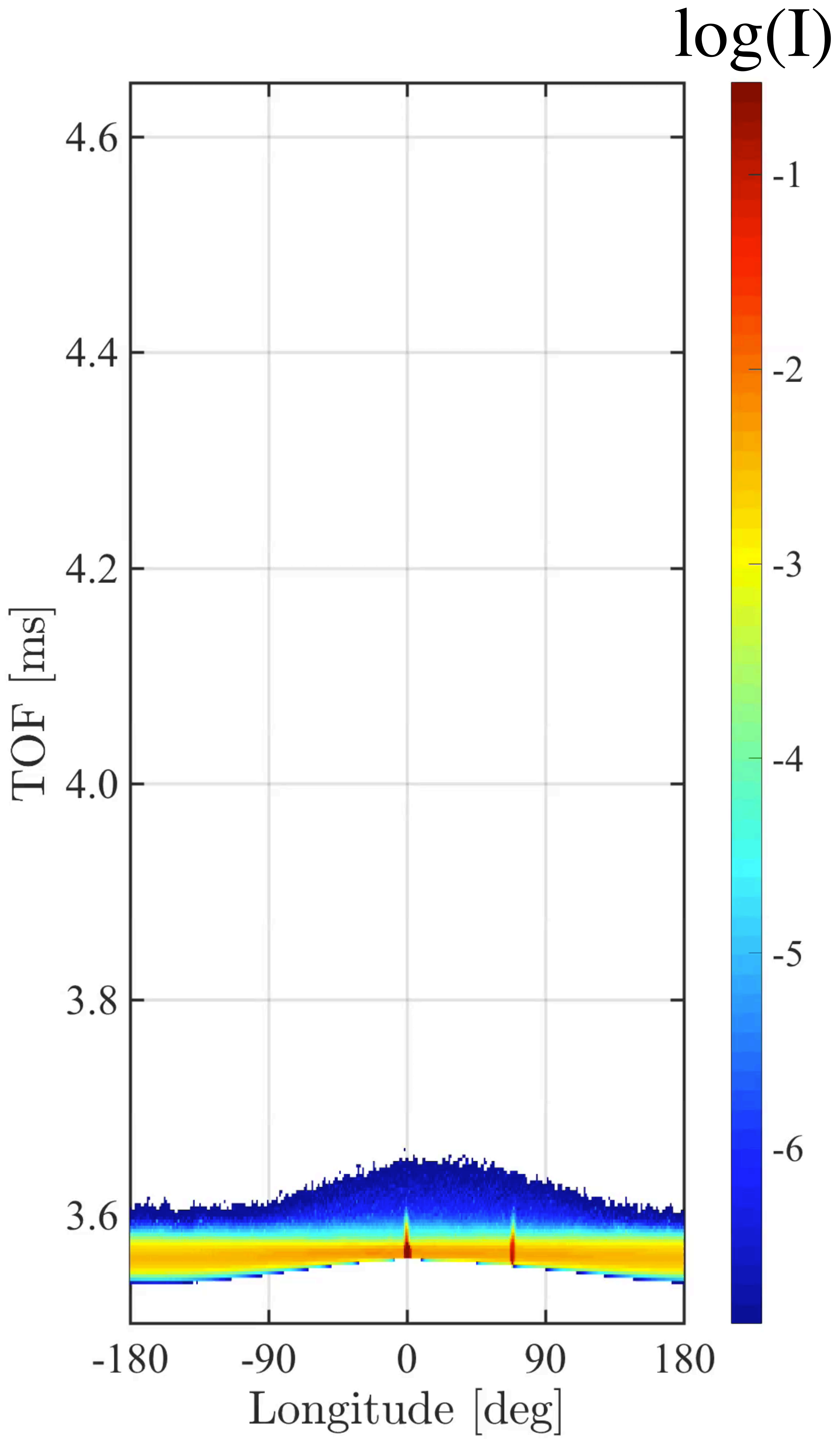

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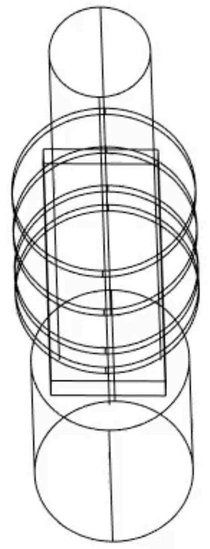

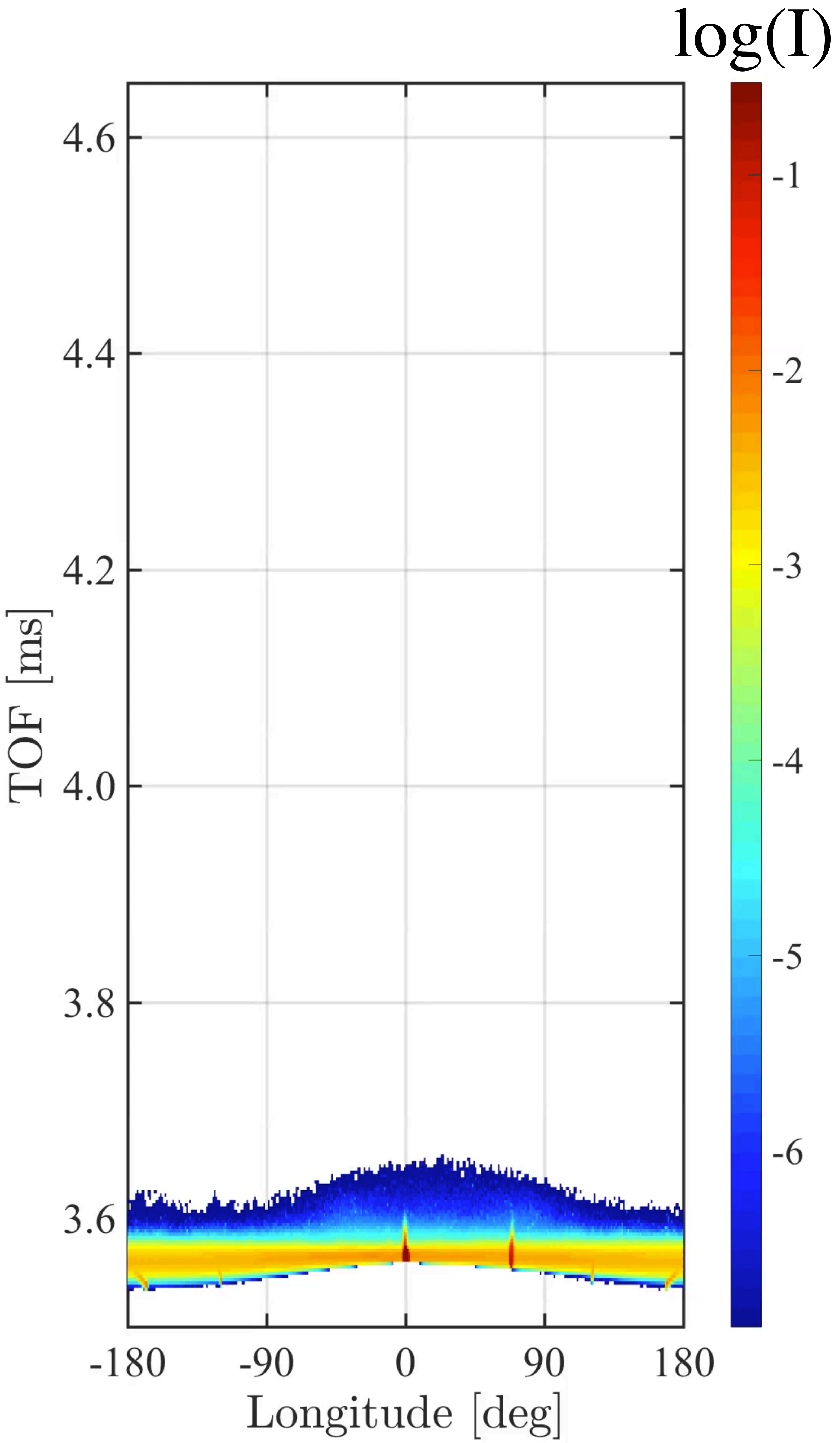

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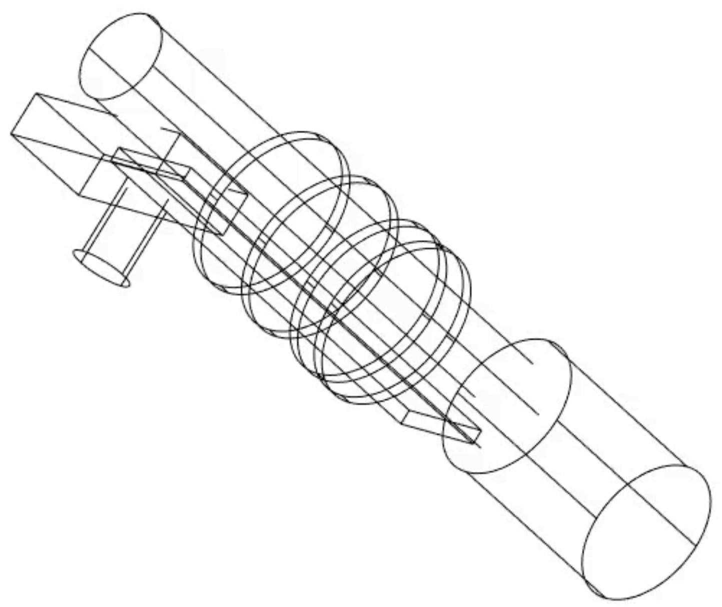

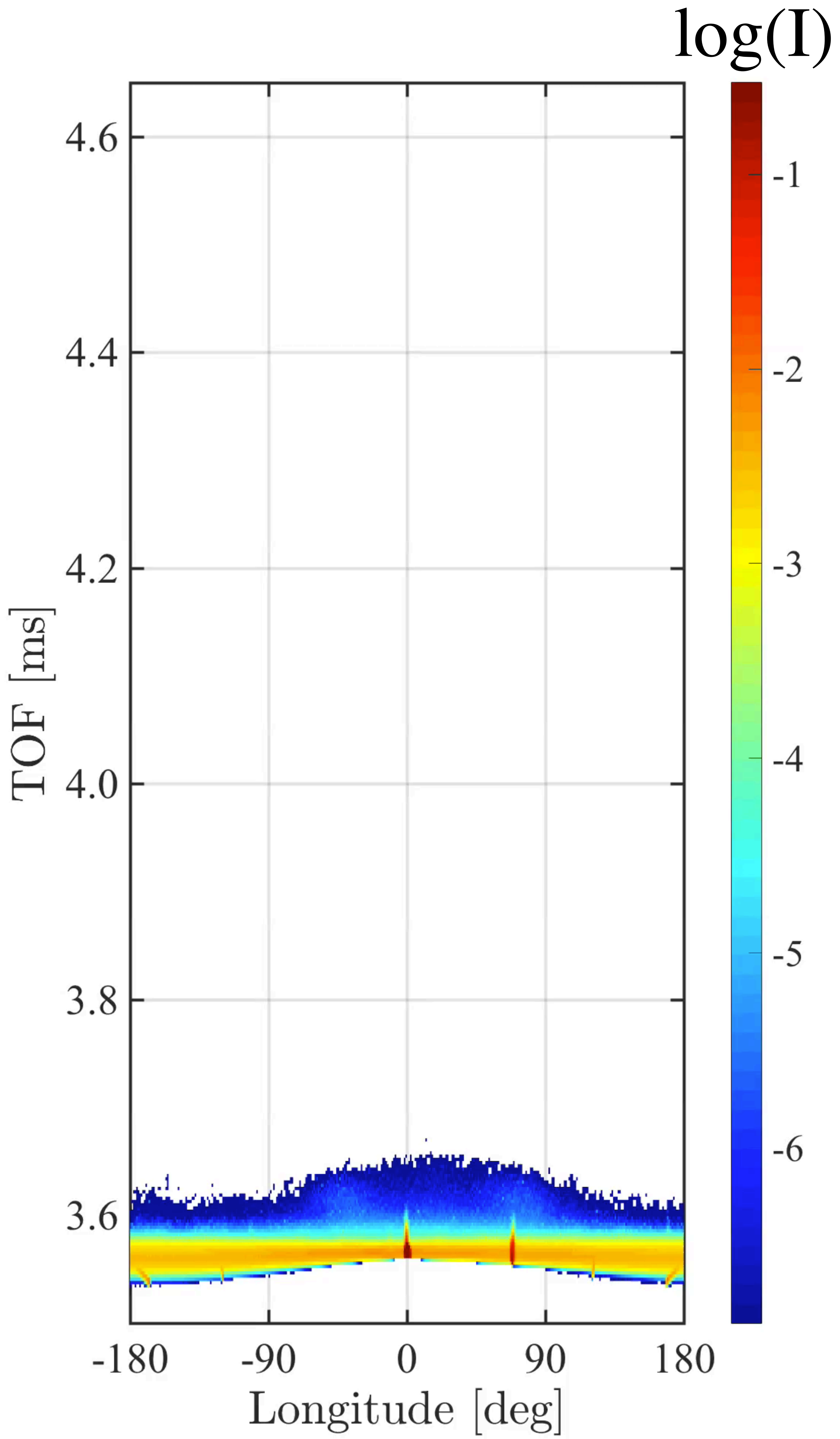

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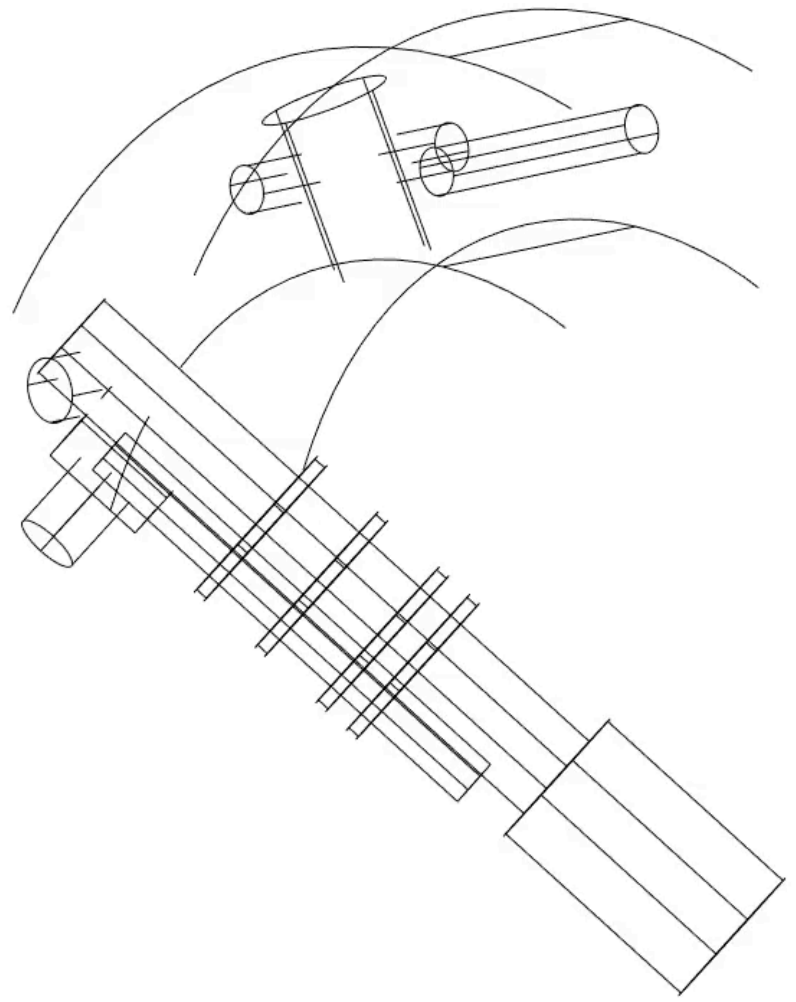

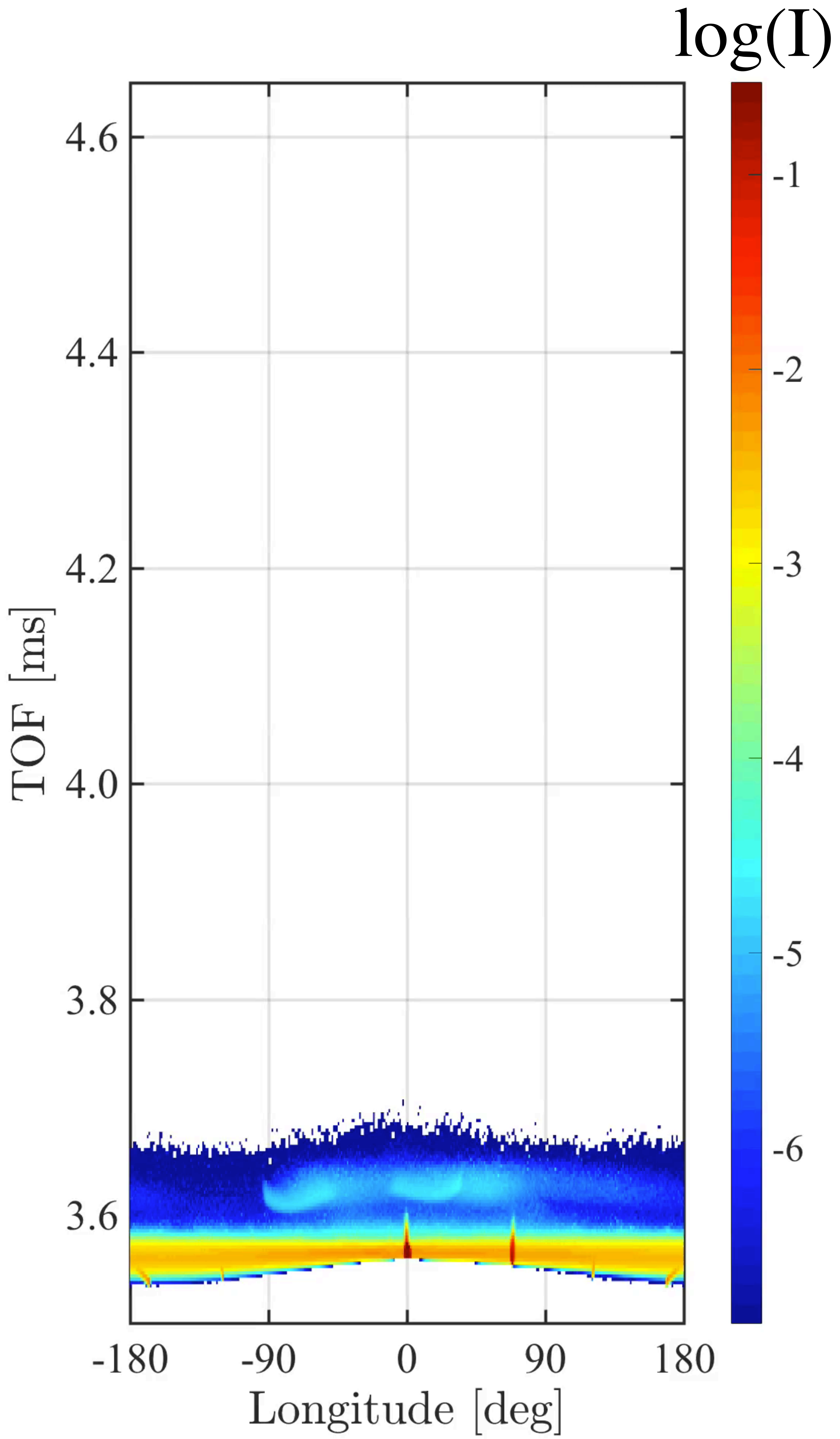

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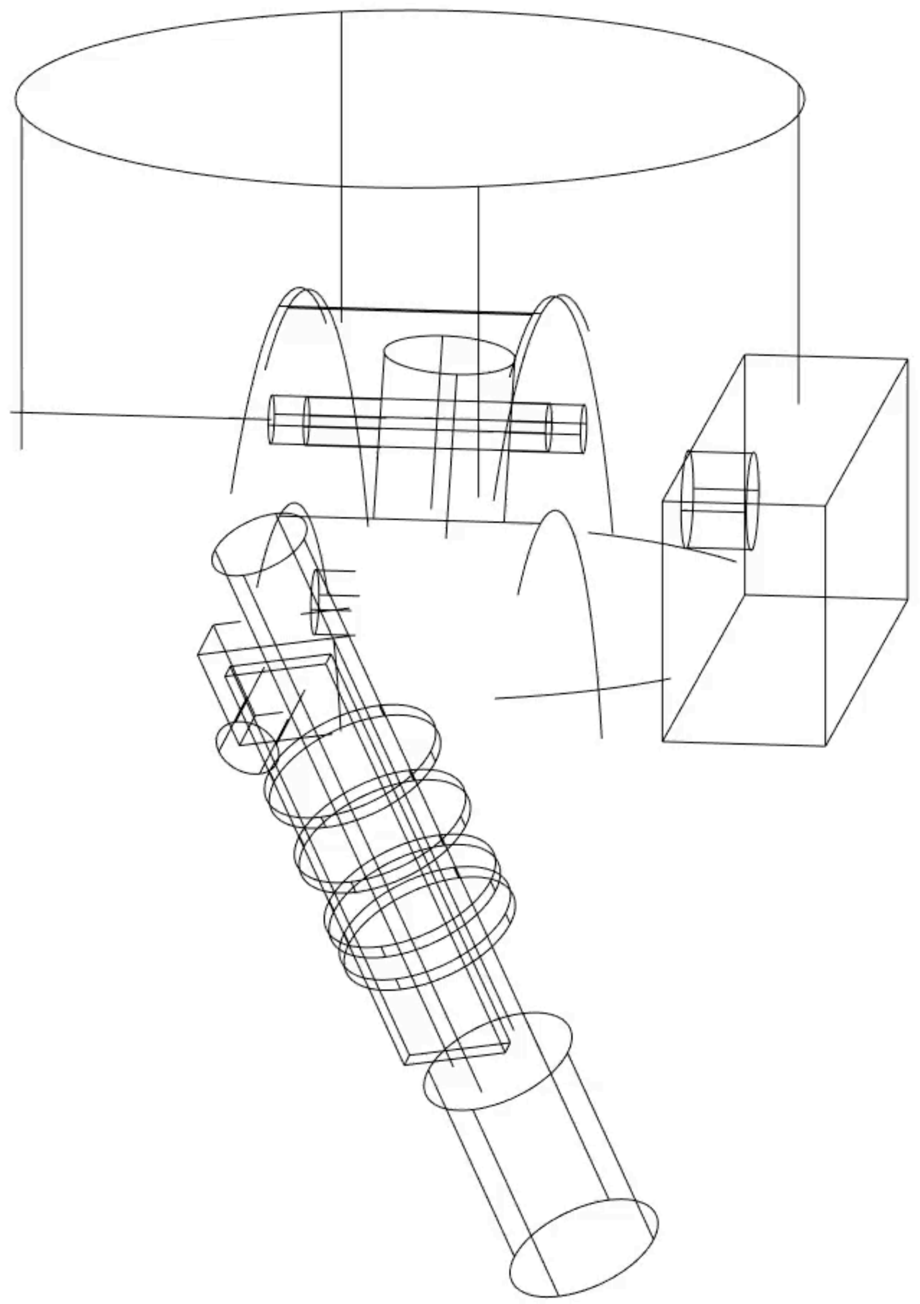

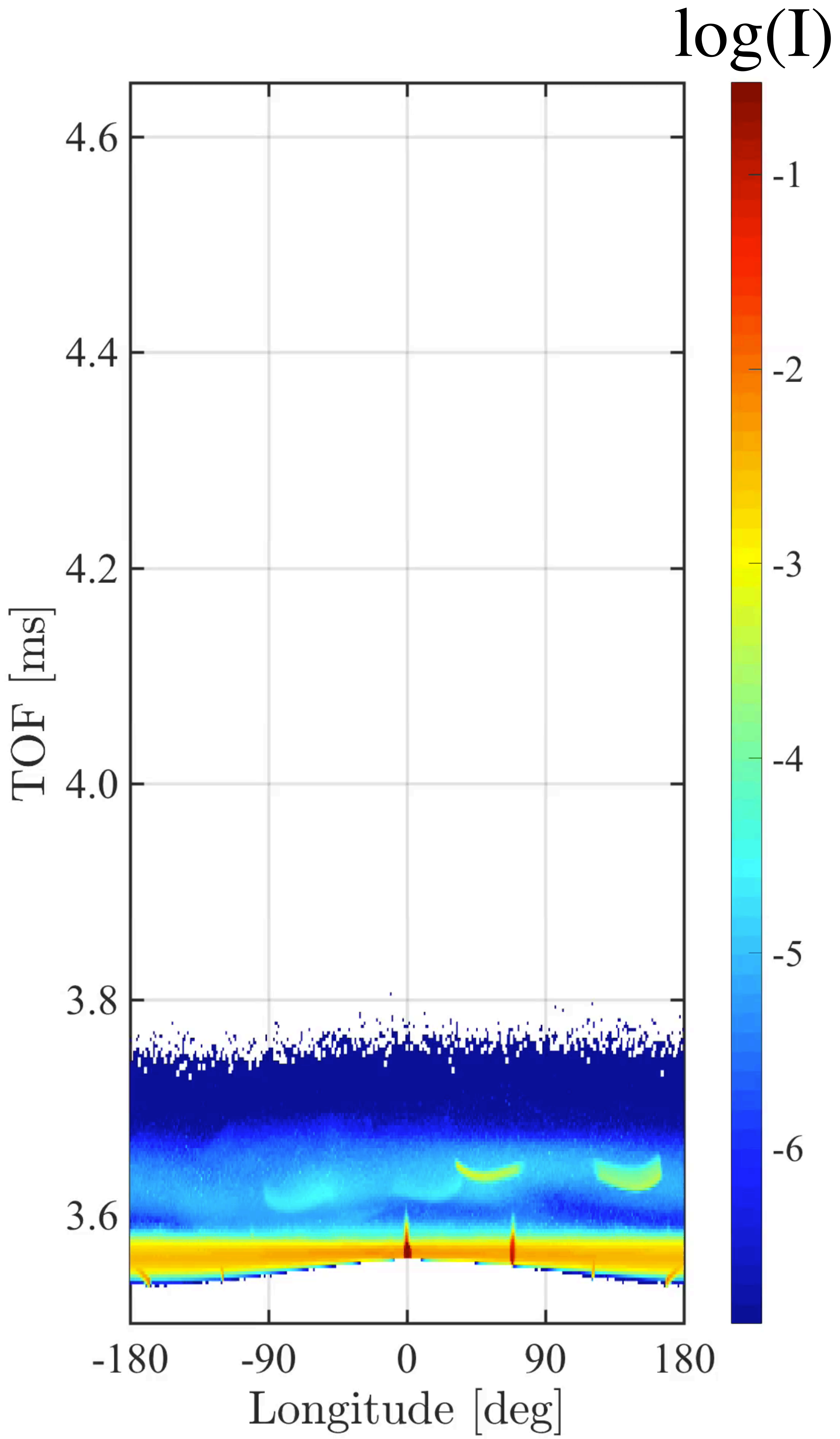

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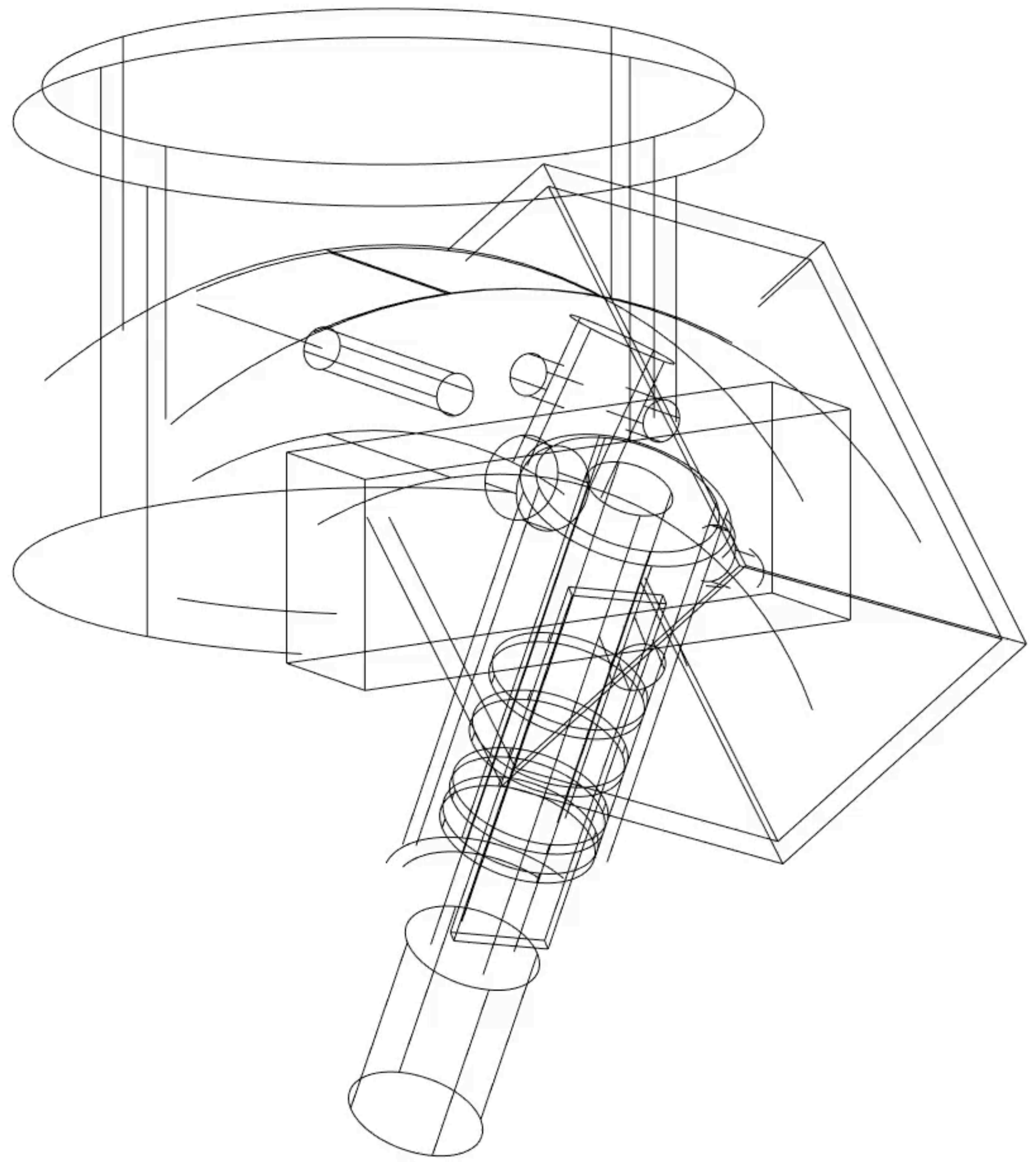

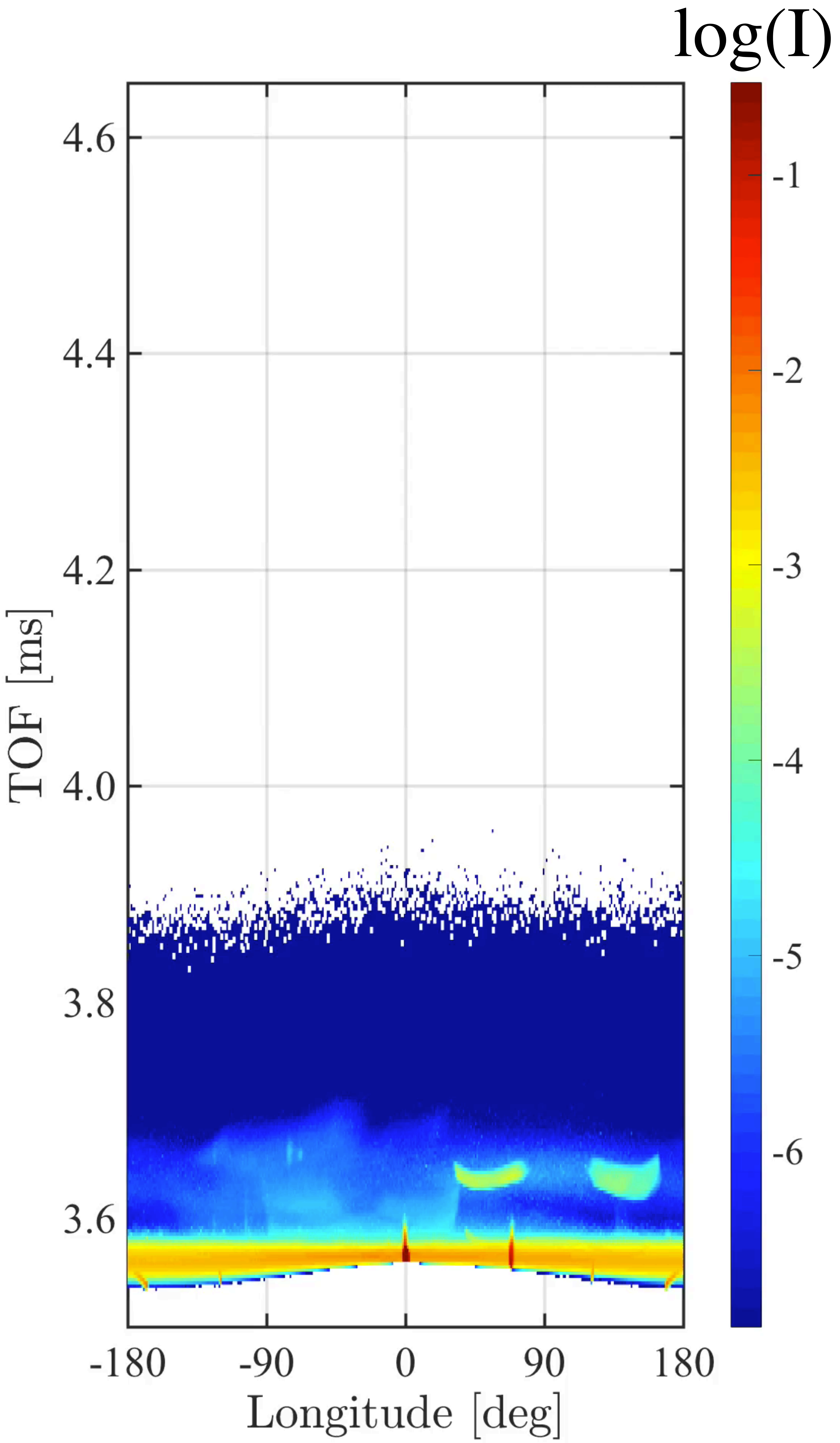

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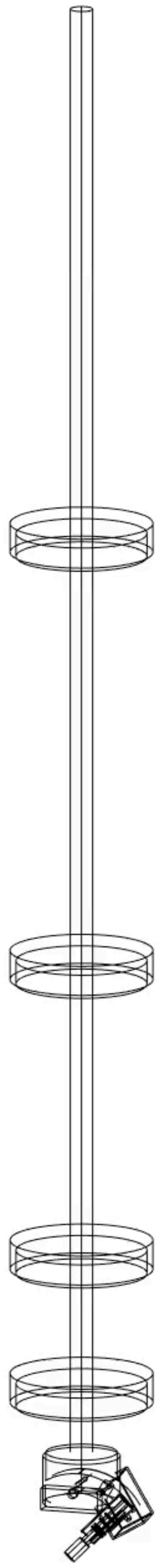

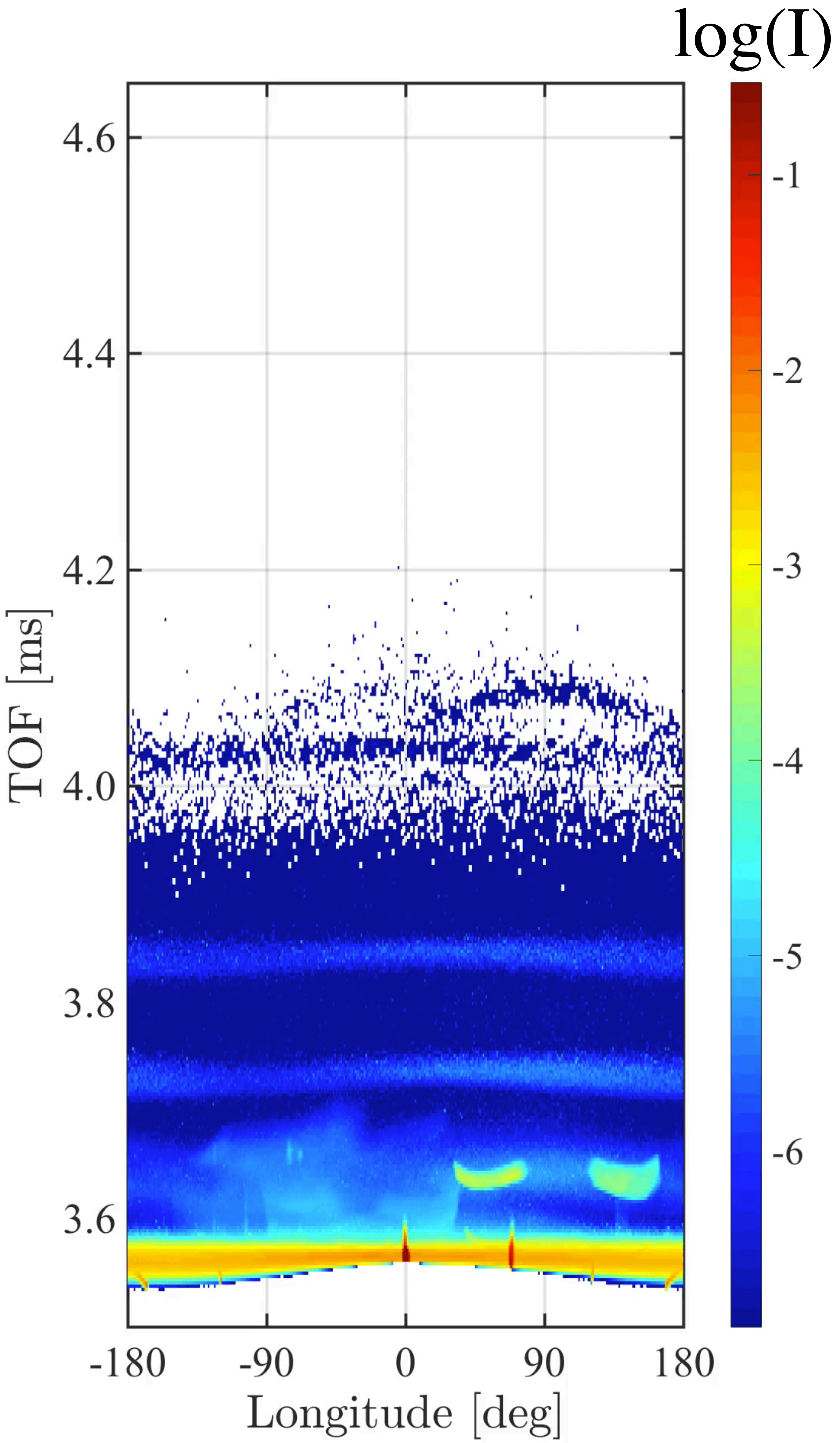

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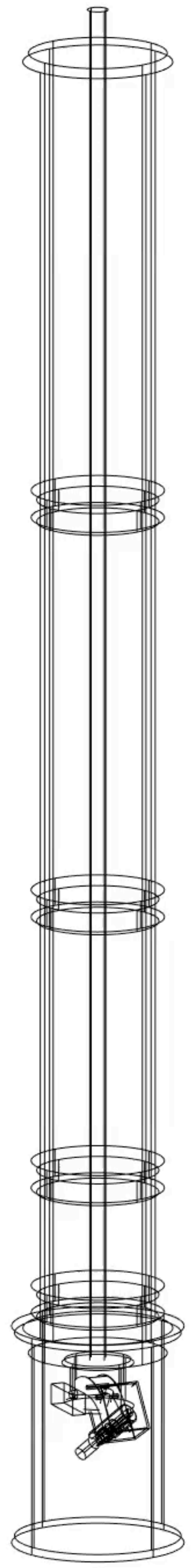

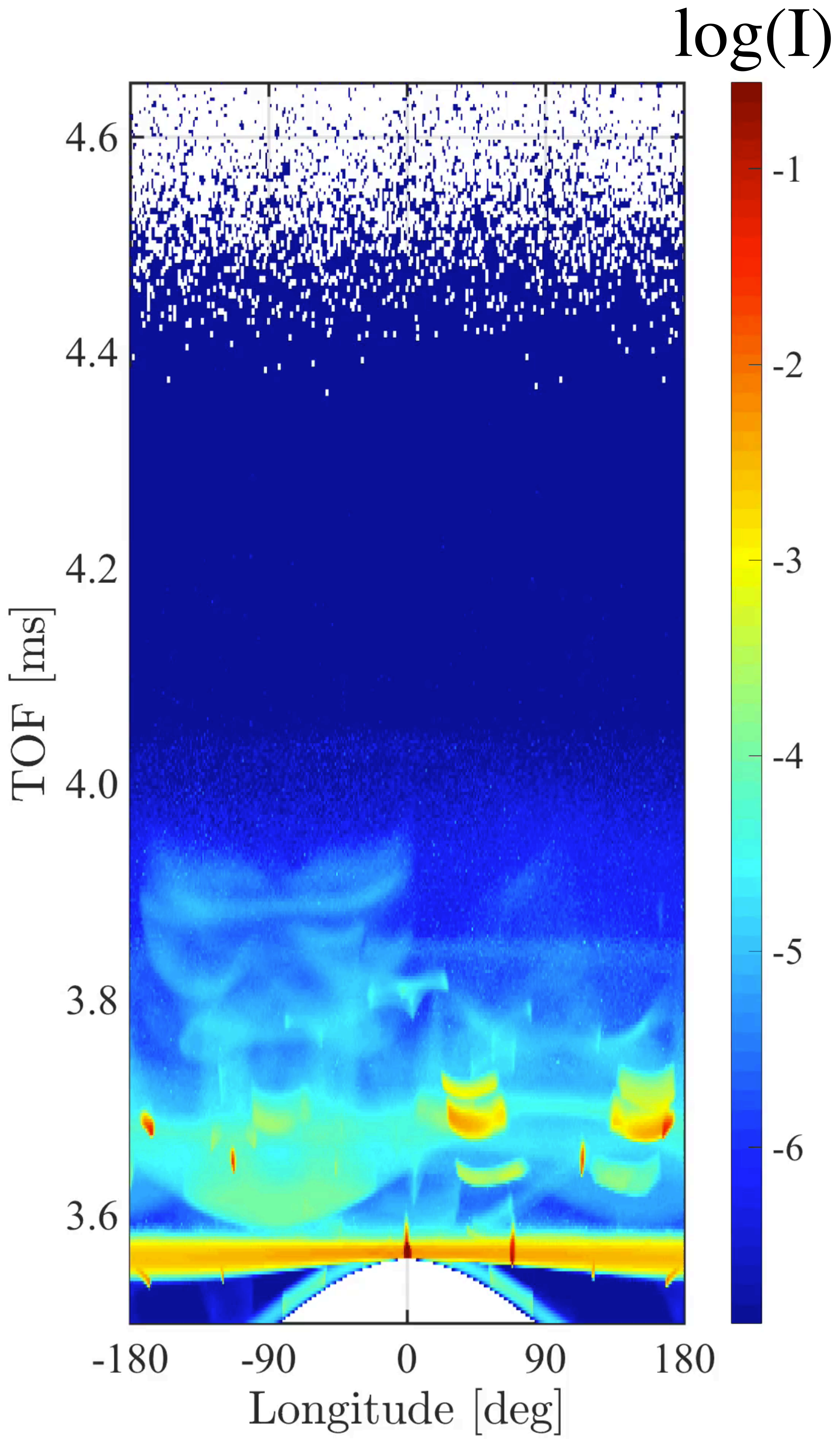

Image from NIST webpage

Building a sample

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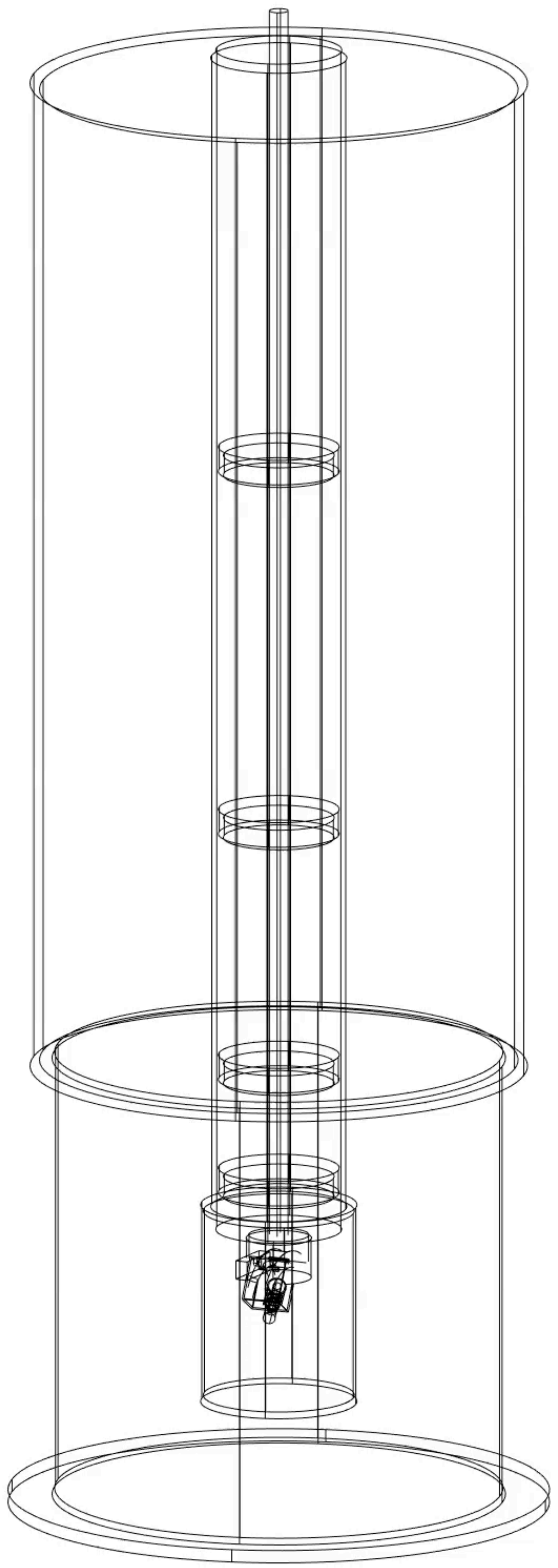
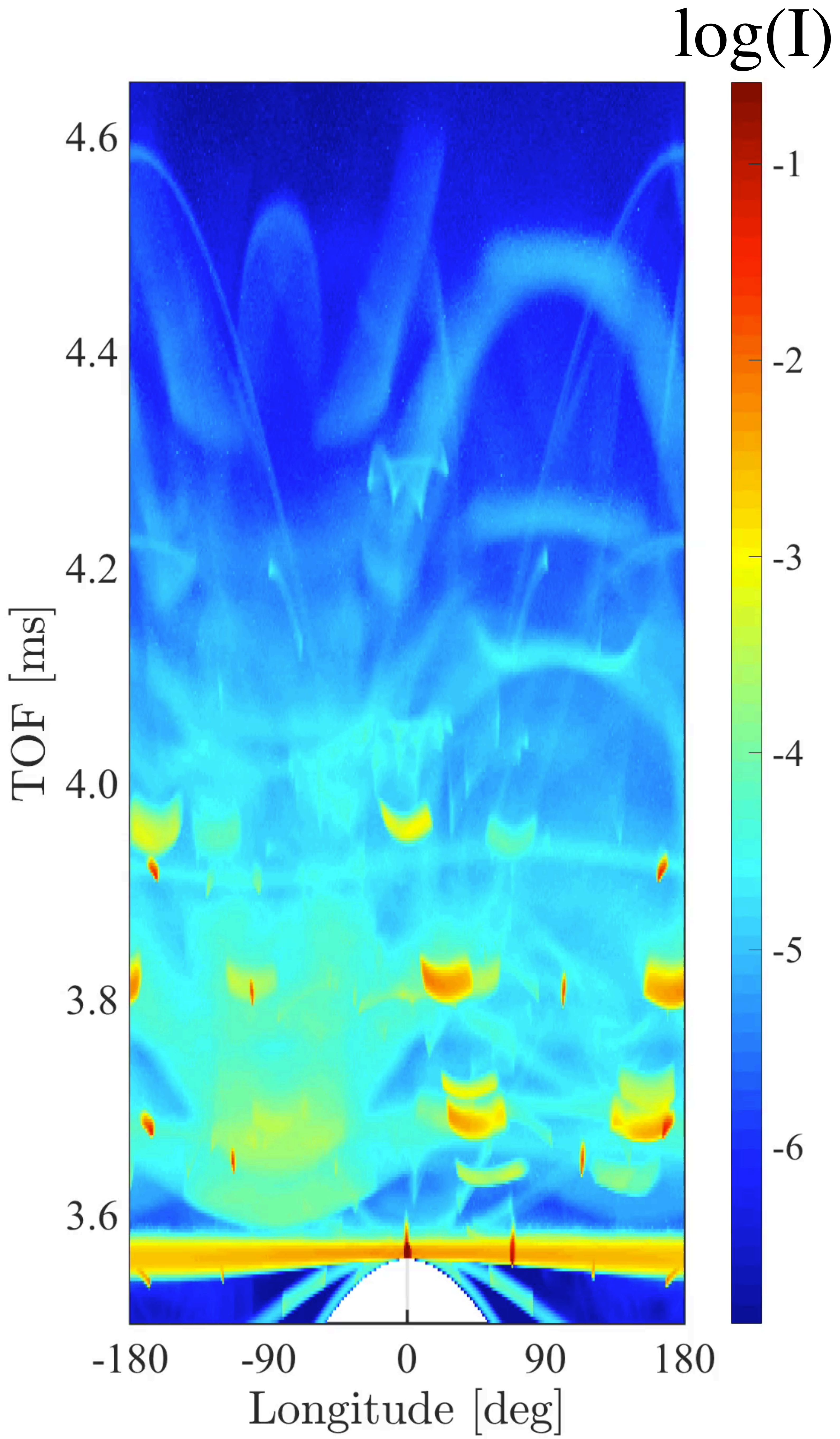
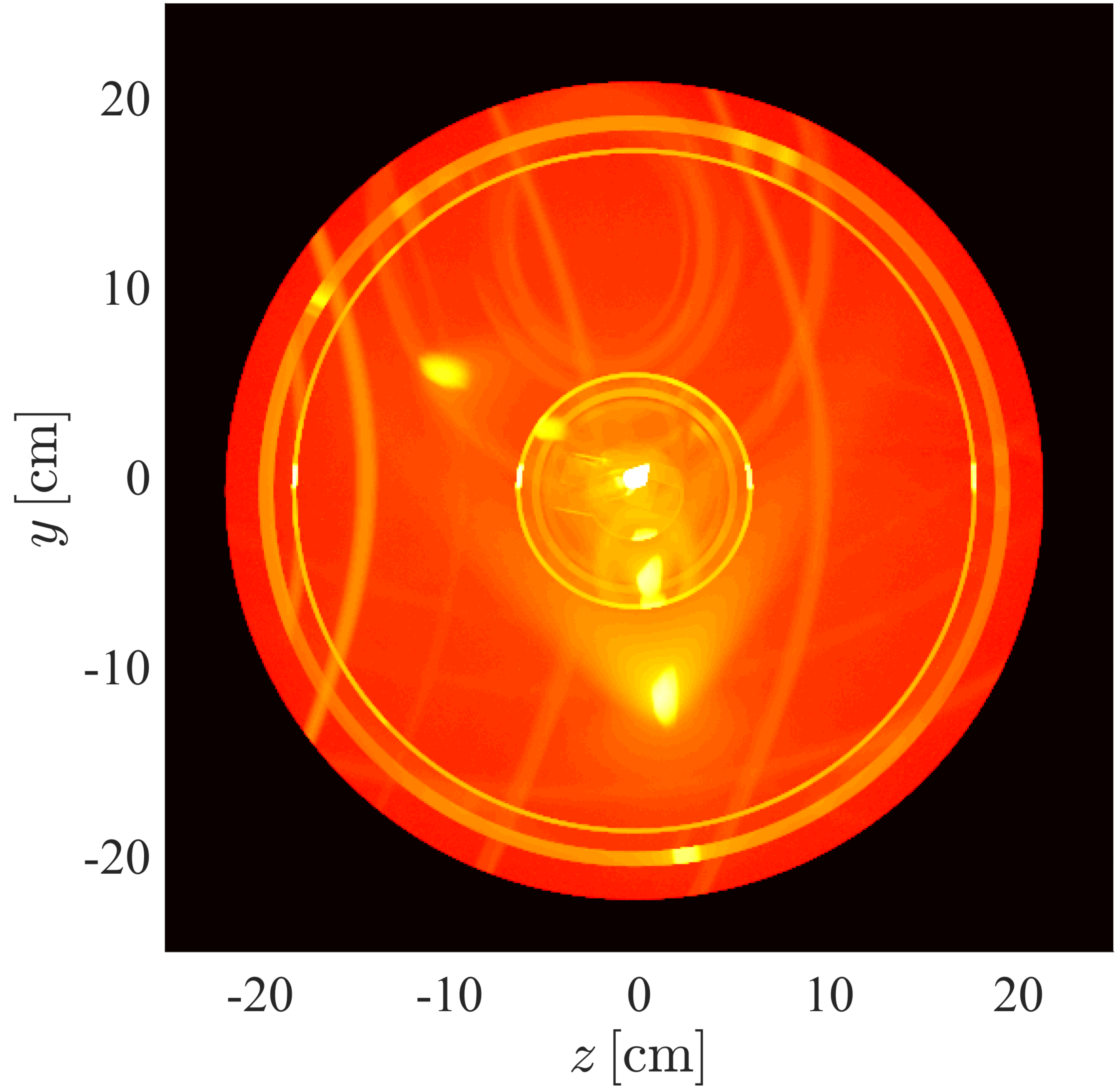




Union loggers

- Loggers can provide insight to what occurred during a simulation
- Here scattered intensity viewed from above the cryostat



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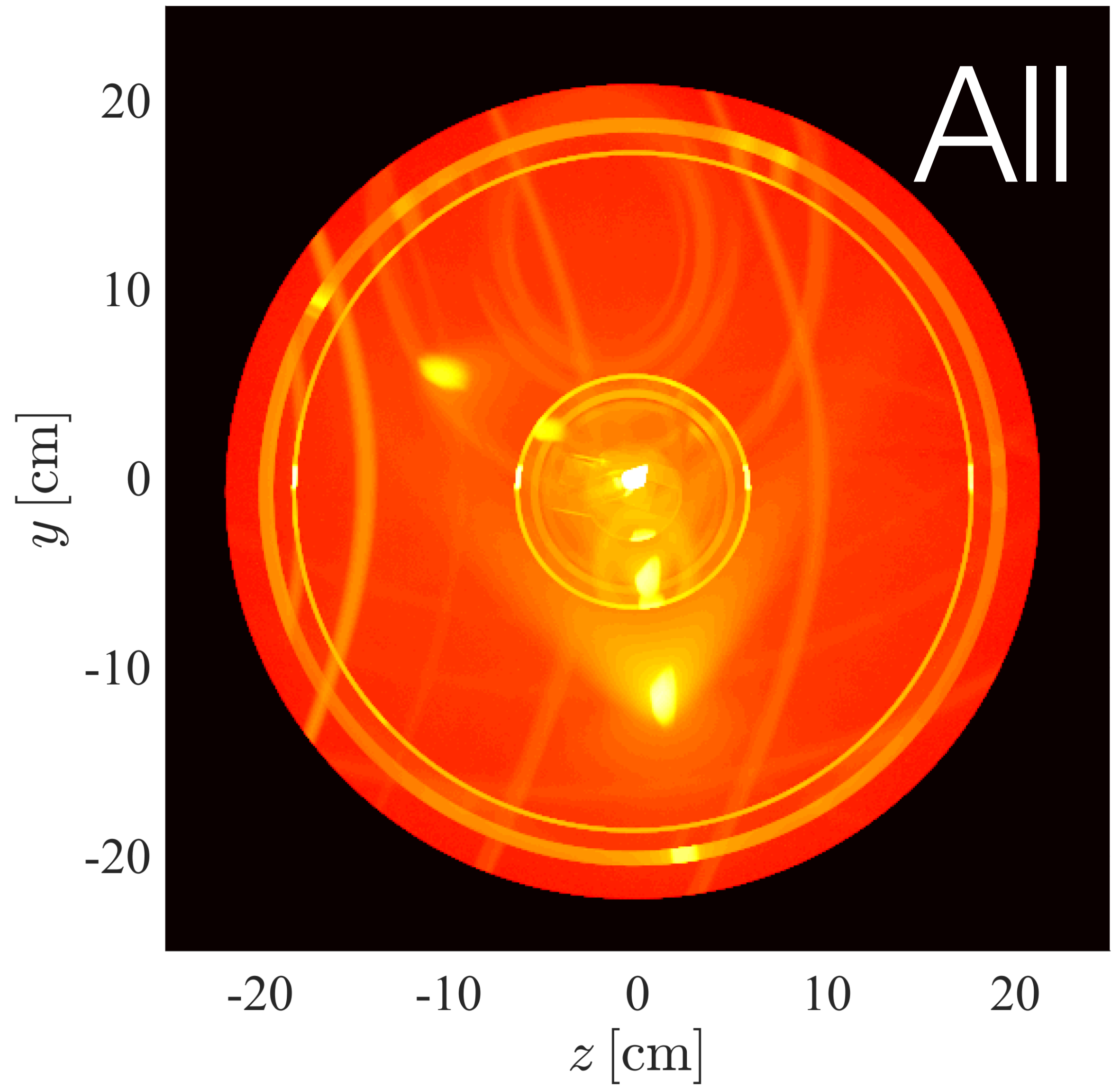
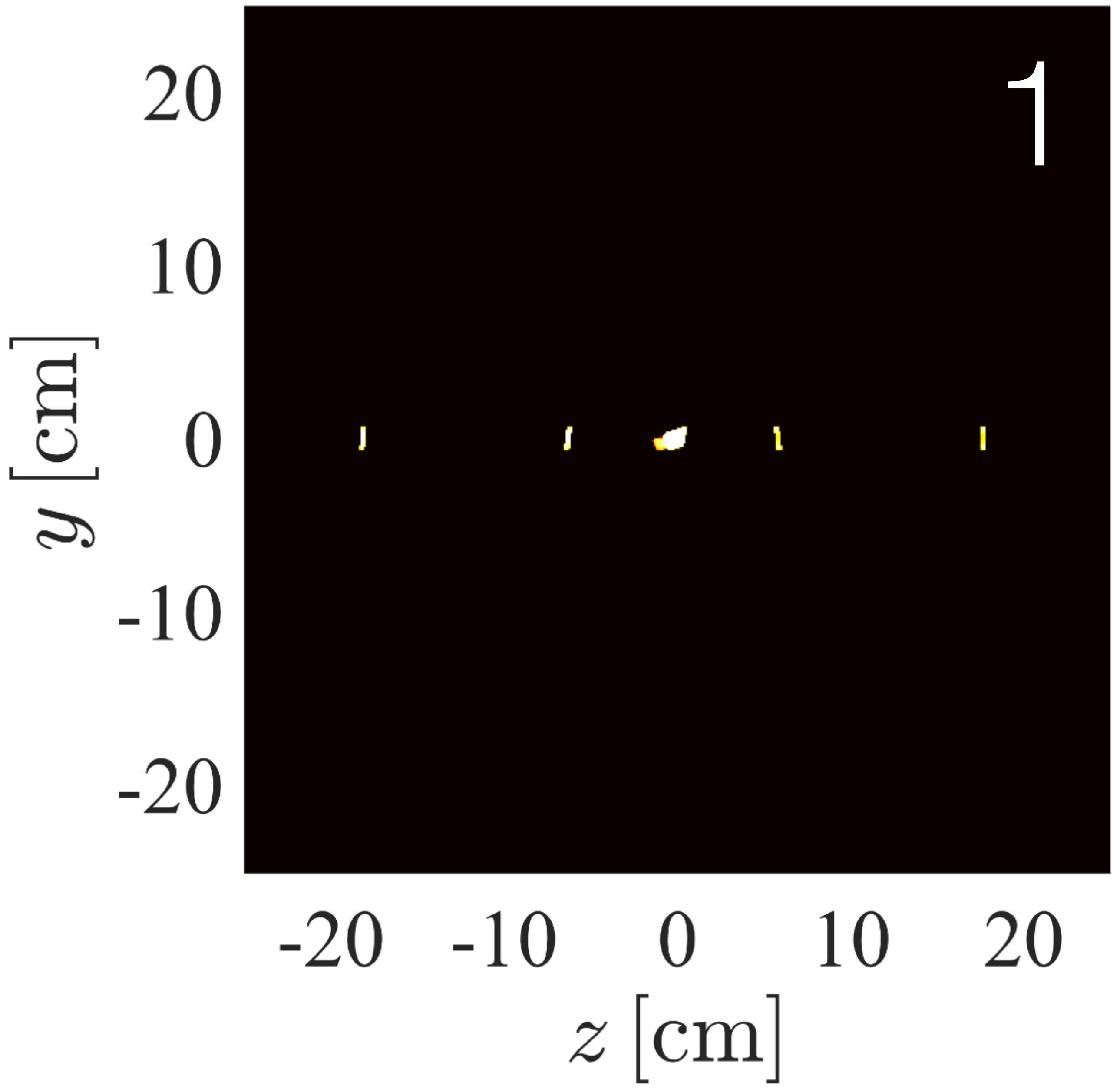
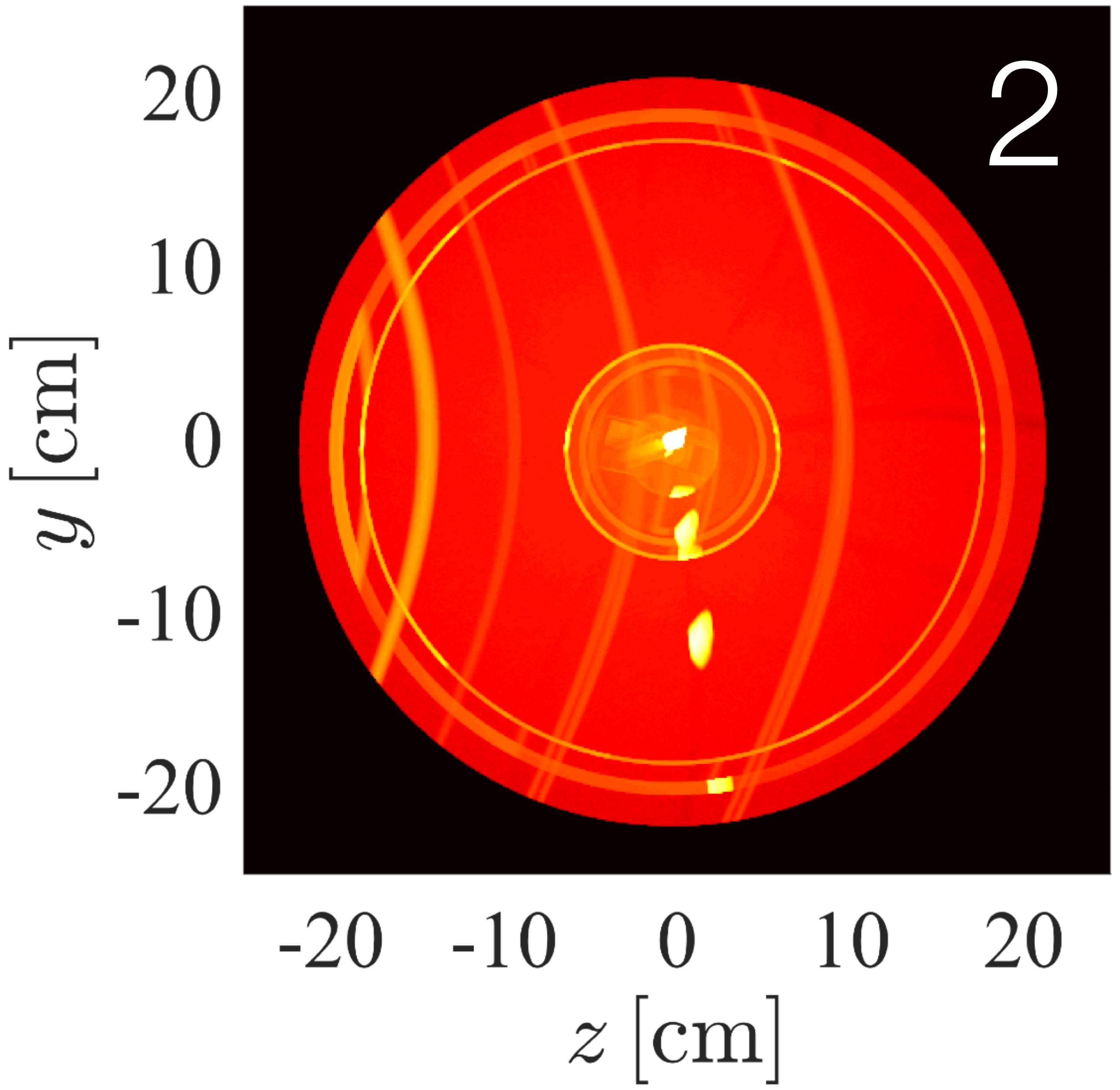
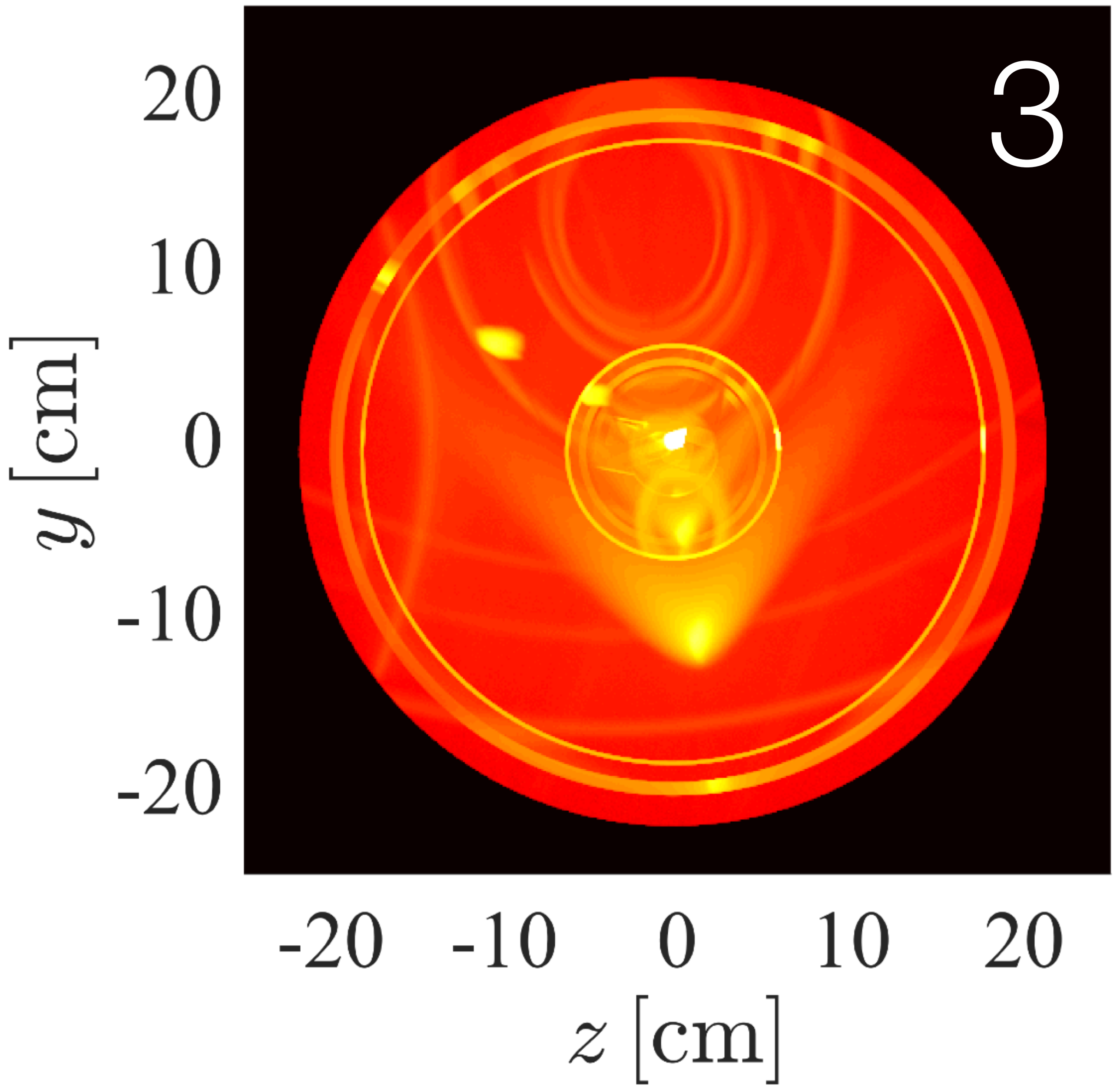


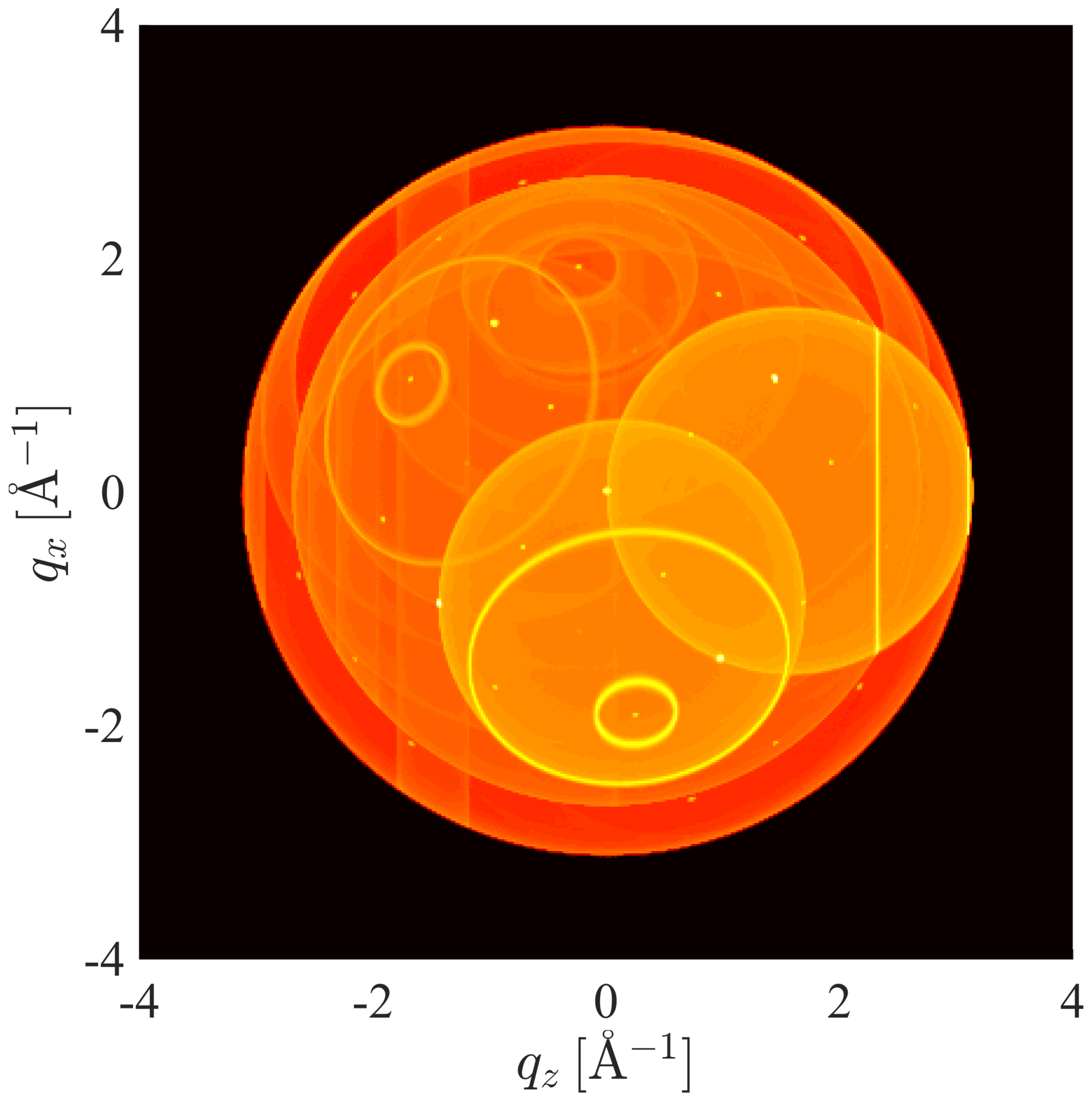






Union loggers

- Loggers can provide insight to what occurred during a simulation
- Here the scattering vector projected onto the scattering plane



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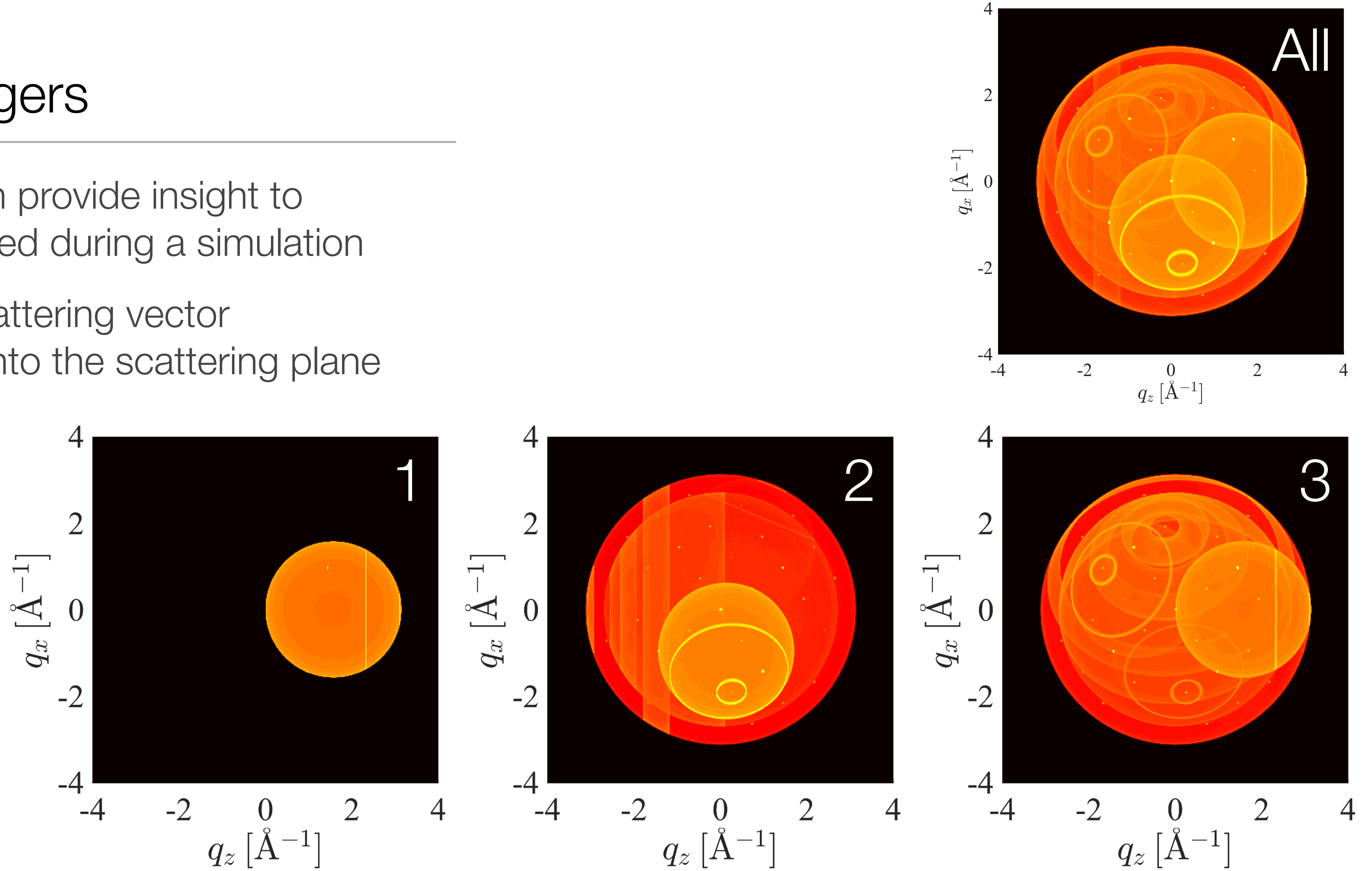
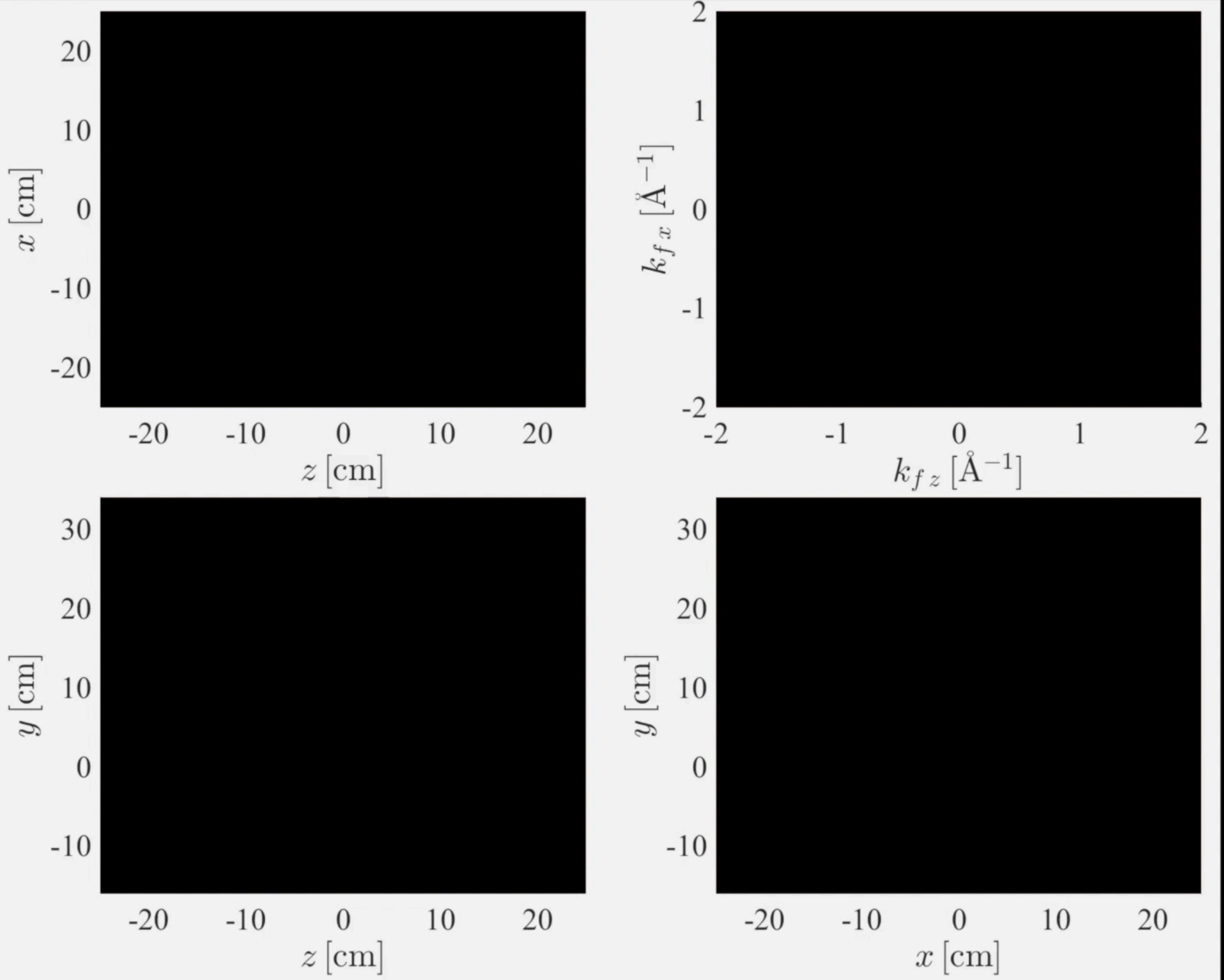
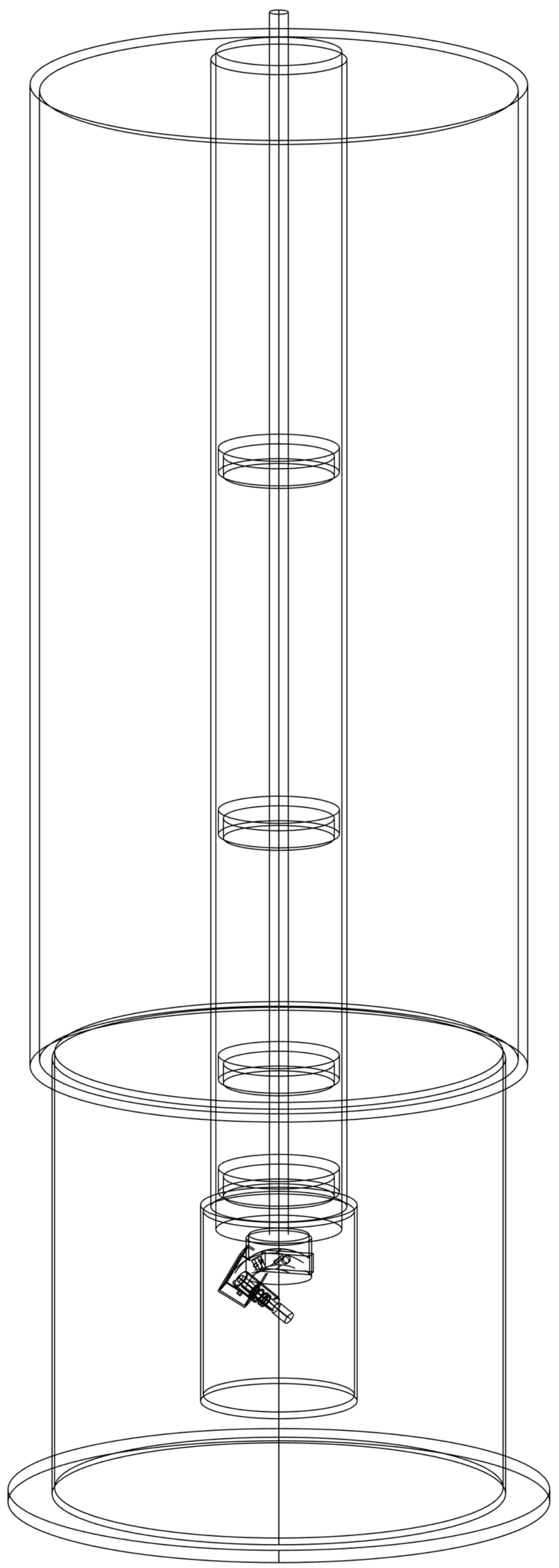


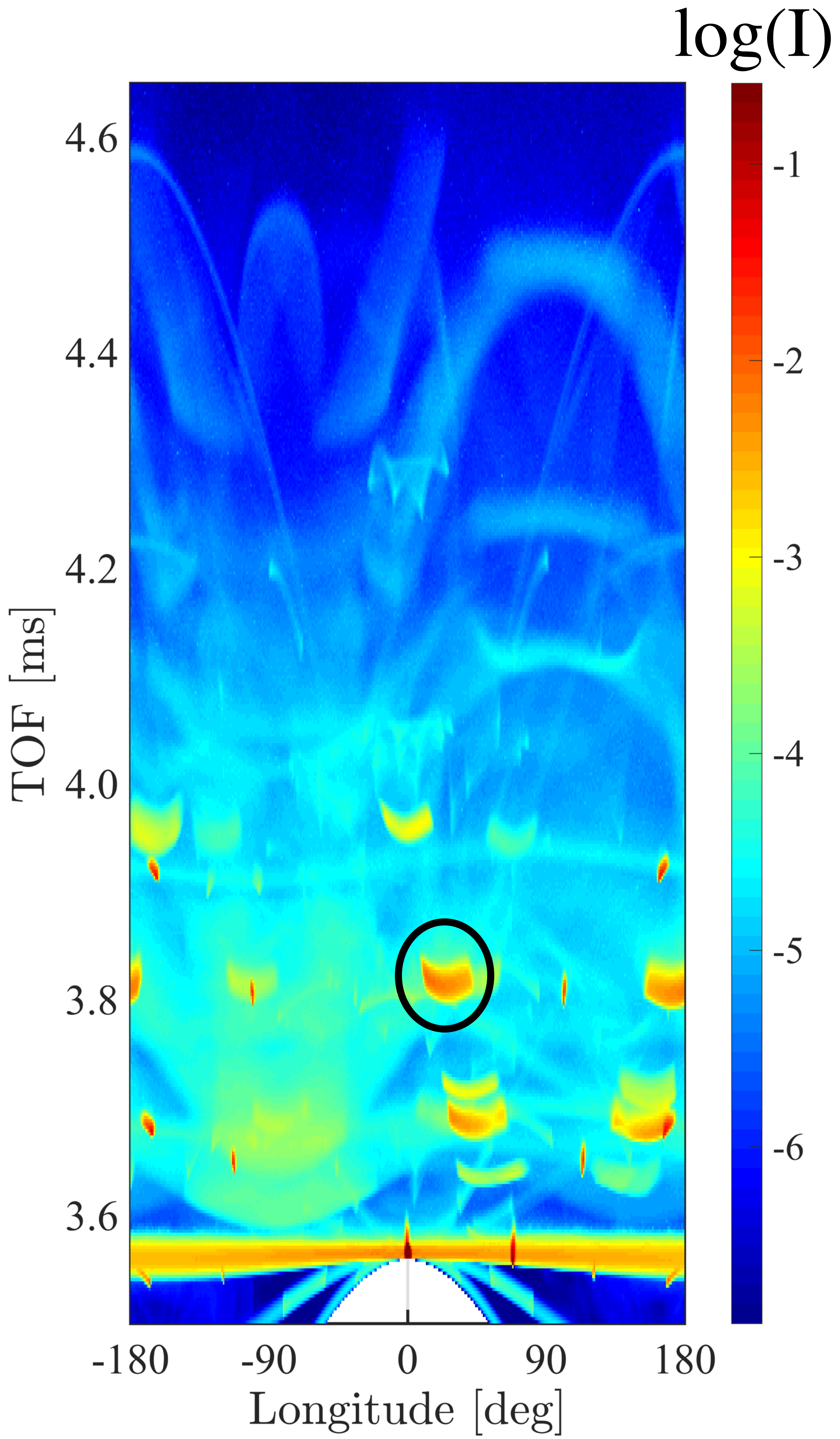


x [cm]
z [cm]
k_{fx} [Å^{-1}]
k_{fz} [Å^{-1}]
y [cm]
z [cm]
y [cm]
x [cm]

McStas Union conditionals

- Necessary to understand origin of specific parts of background
- Union components contains conditional tools





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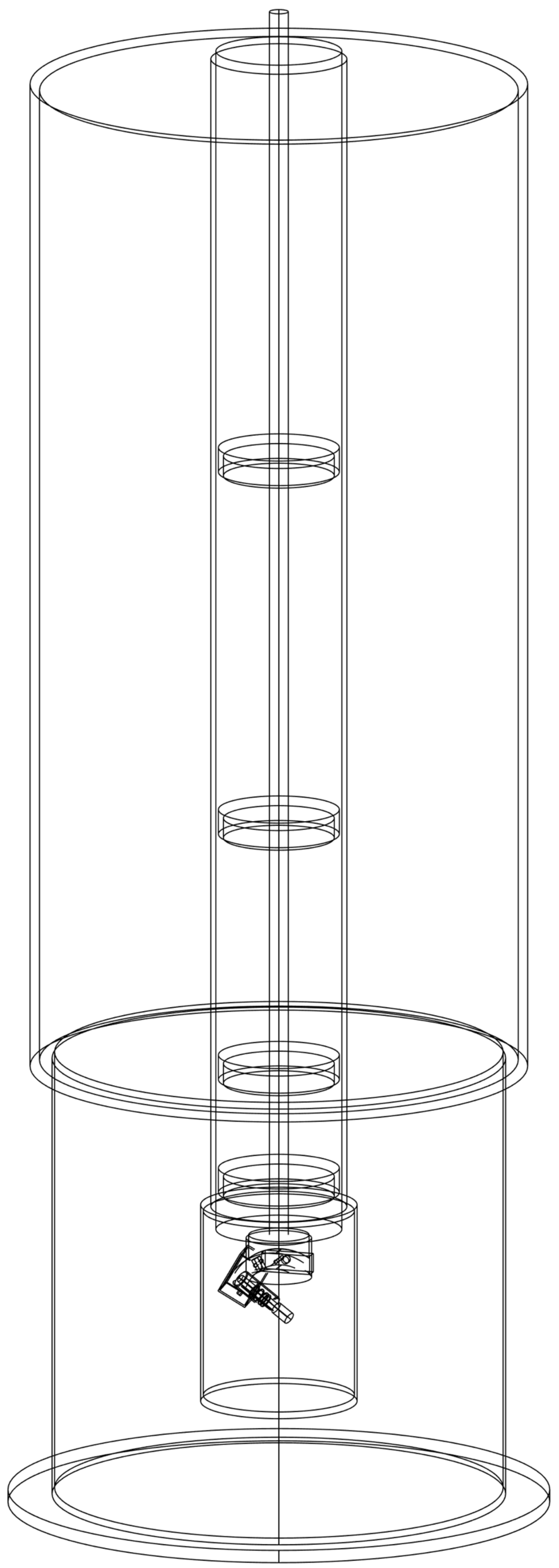
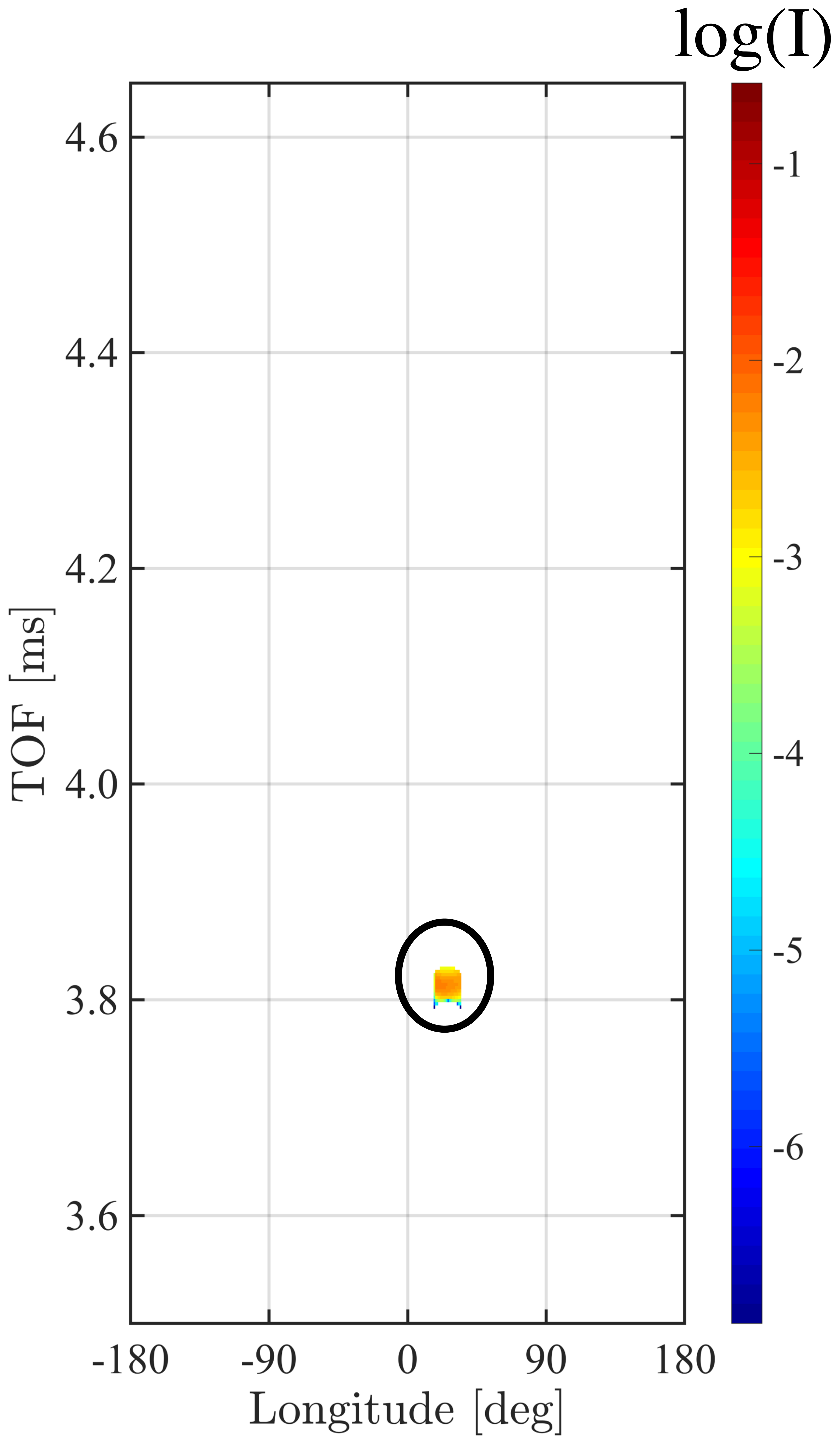
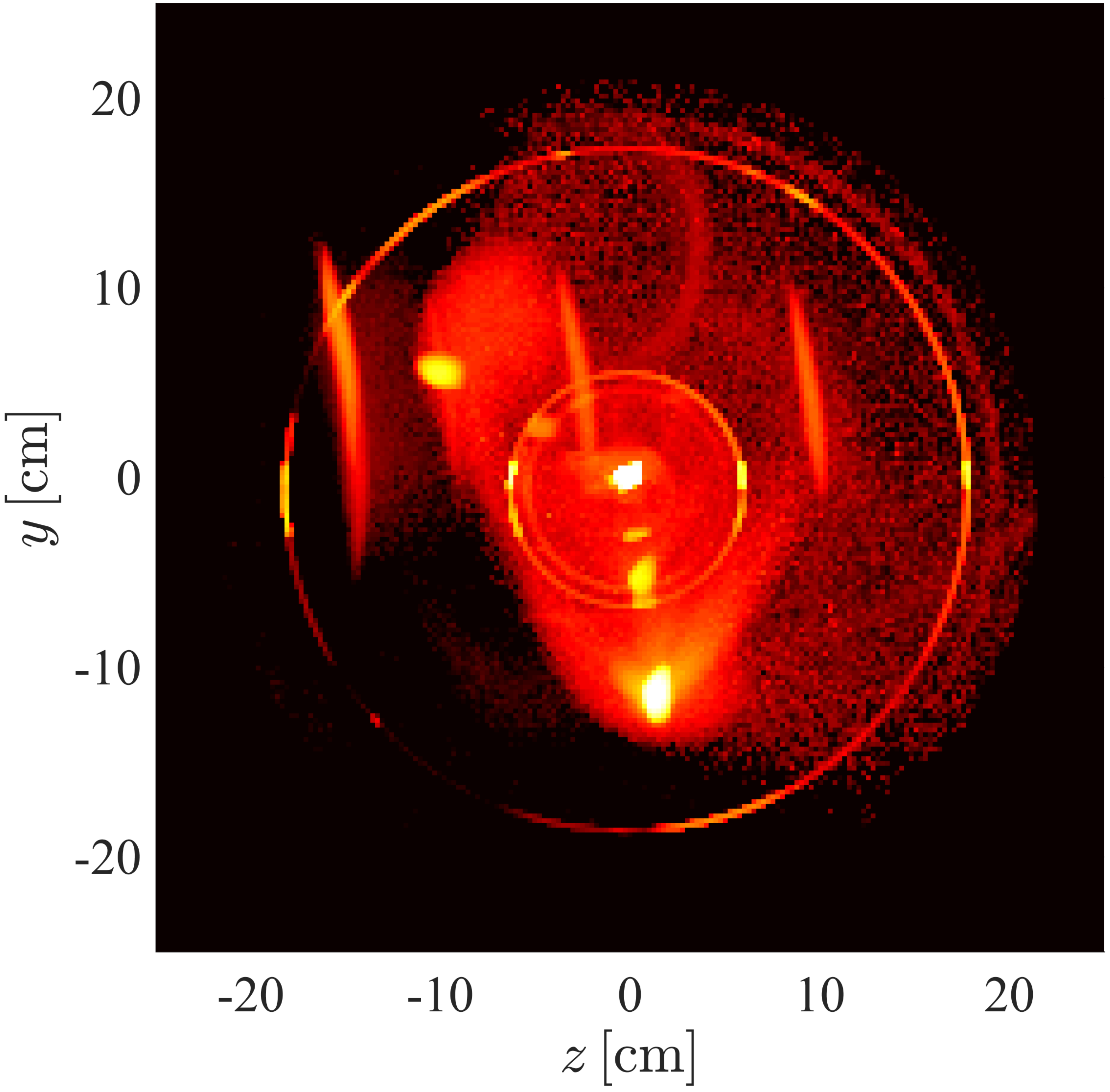




McStas Union conditionals

- Conditionals modify loggers so that only rays with correct final state is recorded
- Here scattering contributing to a certain background event is shown



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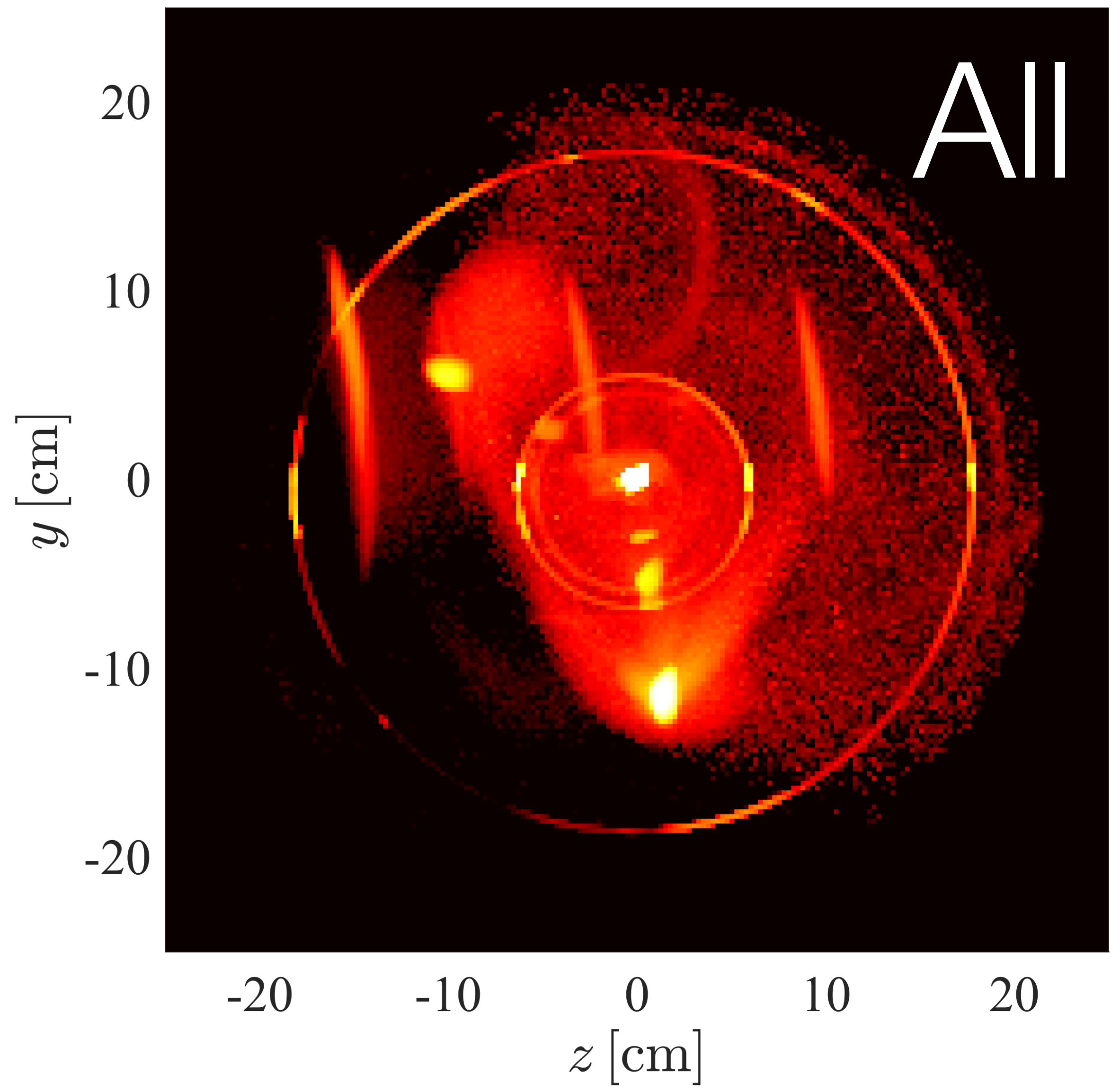

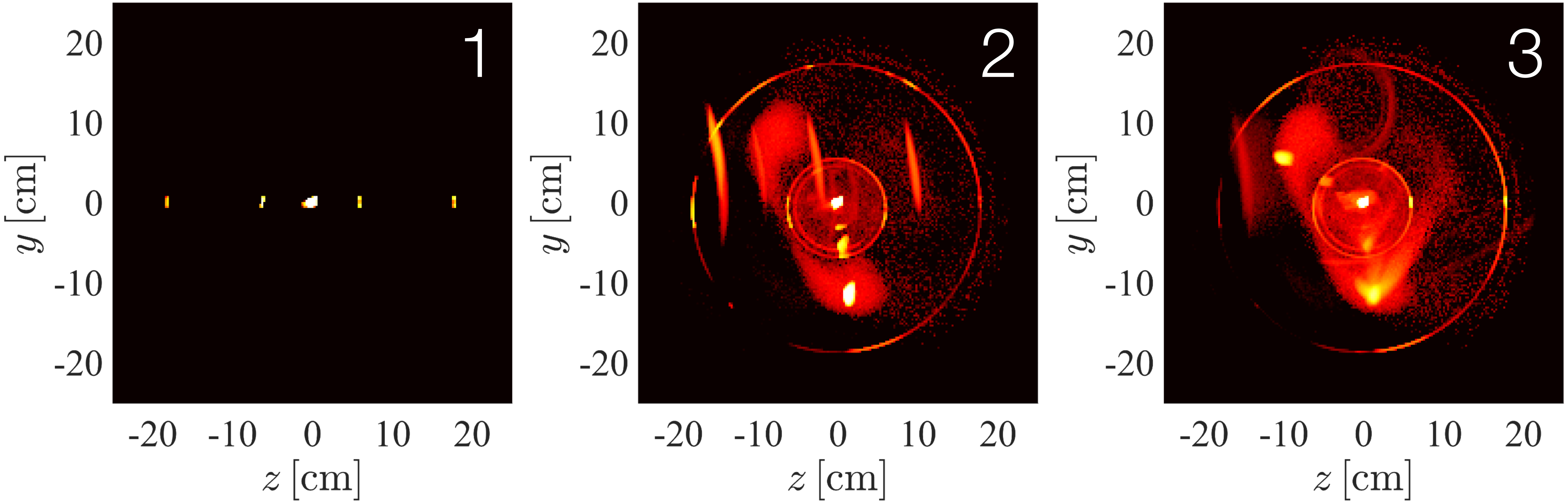

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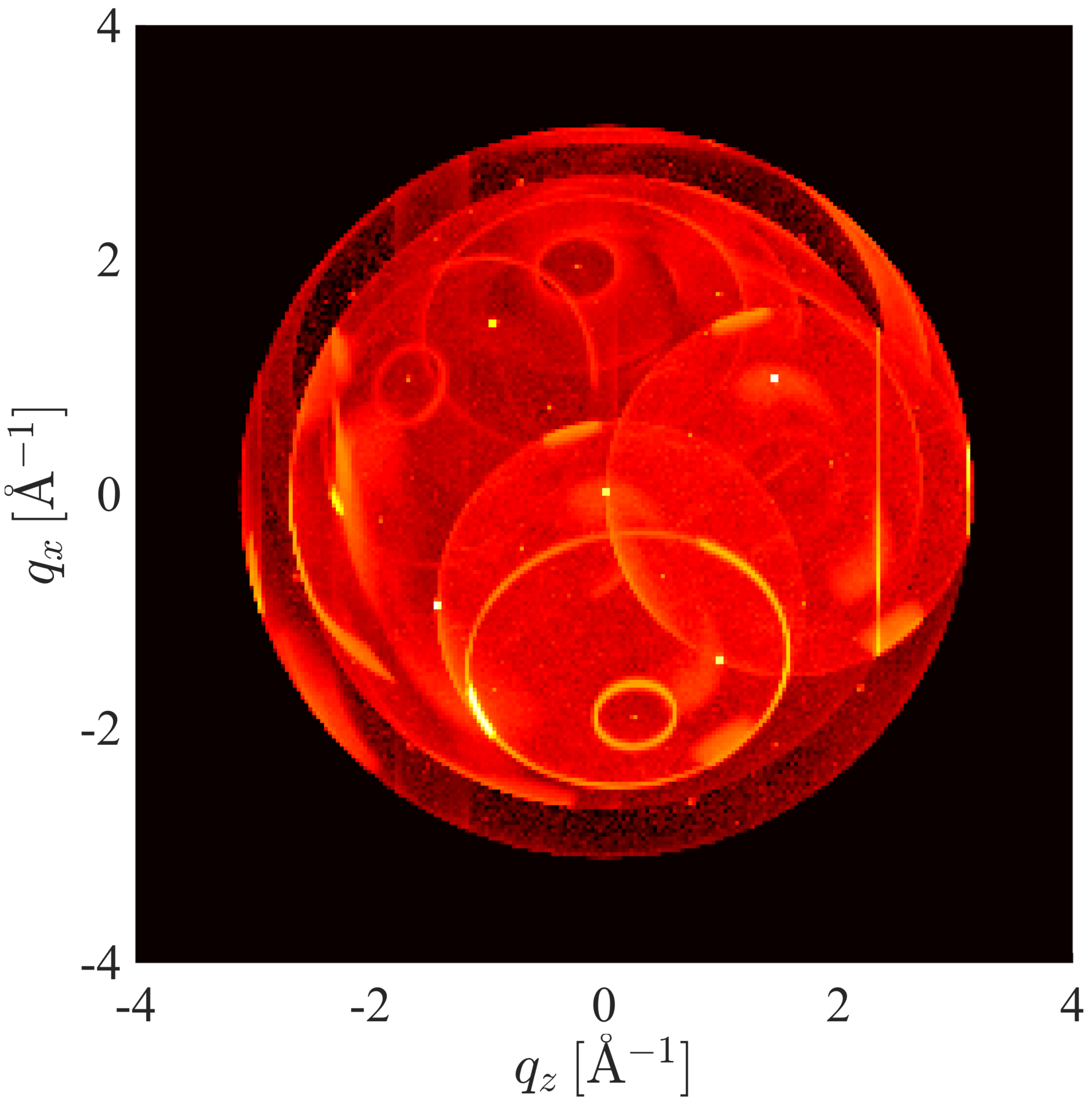

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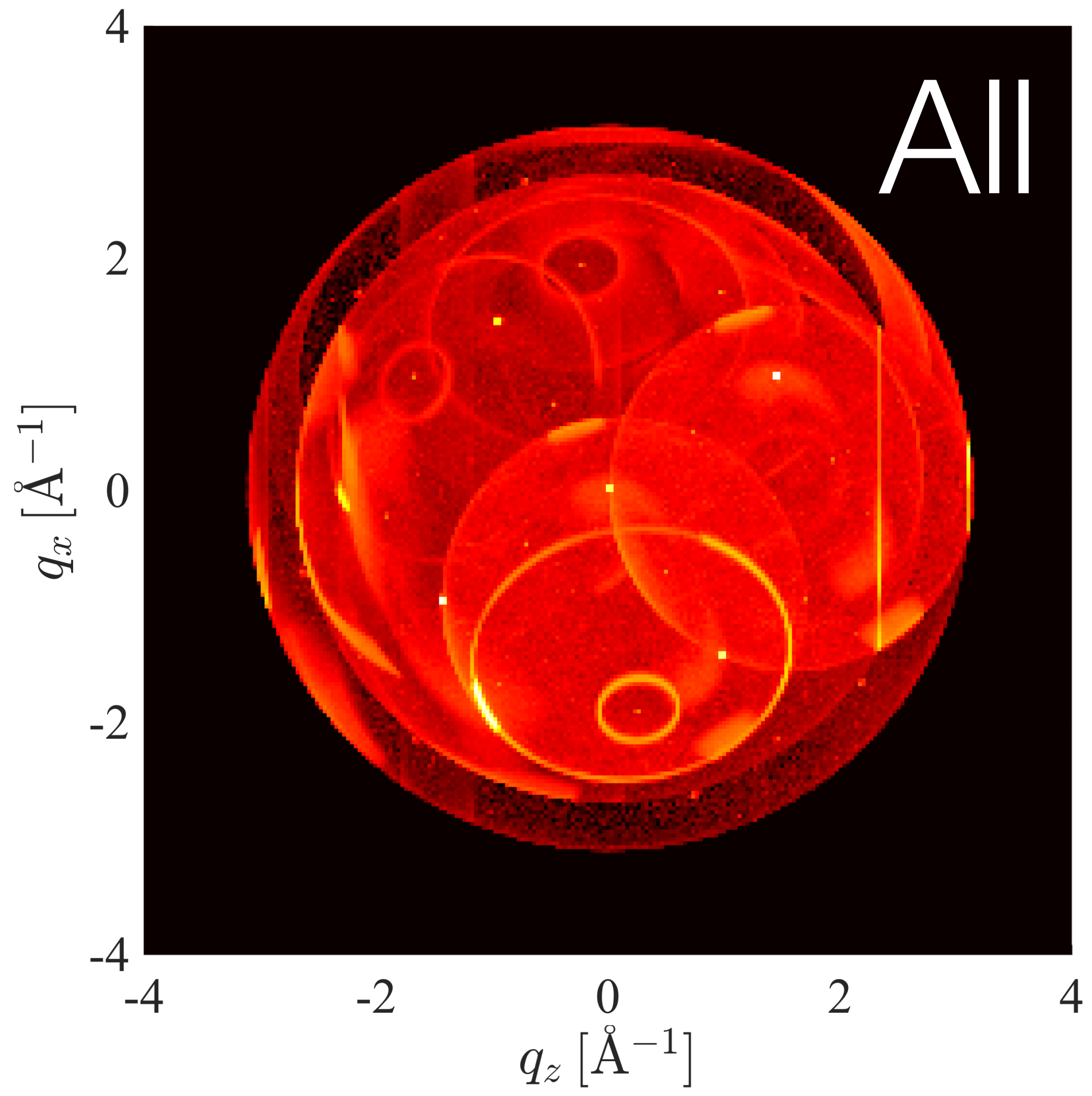
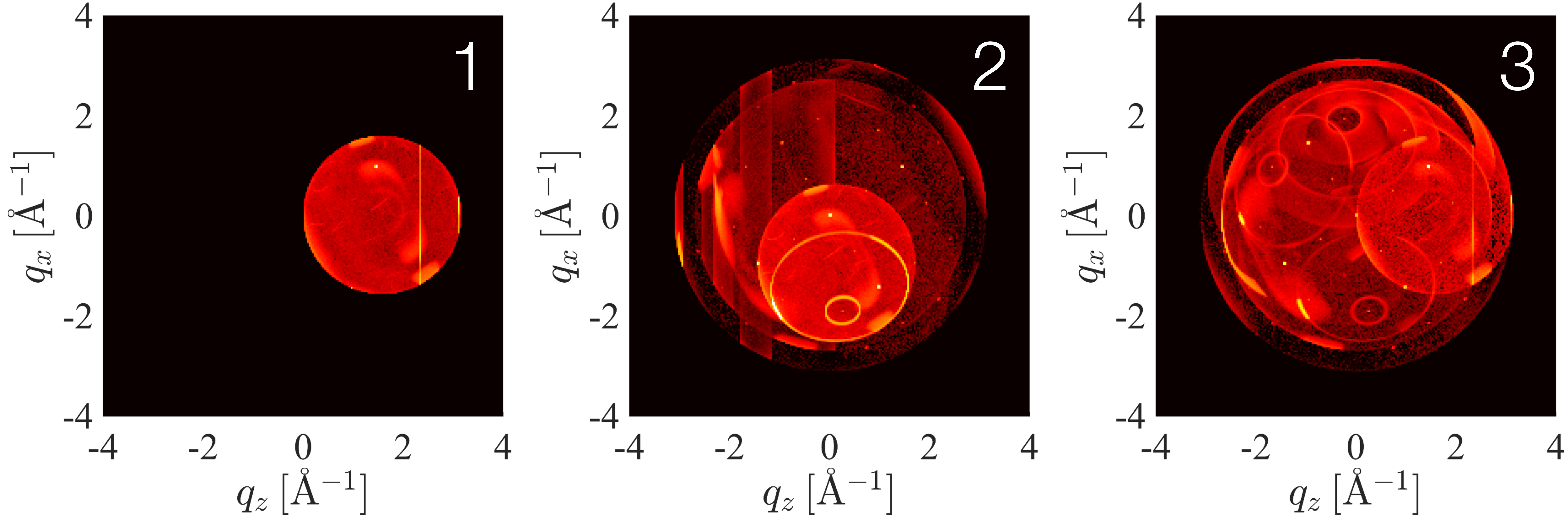
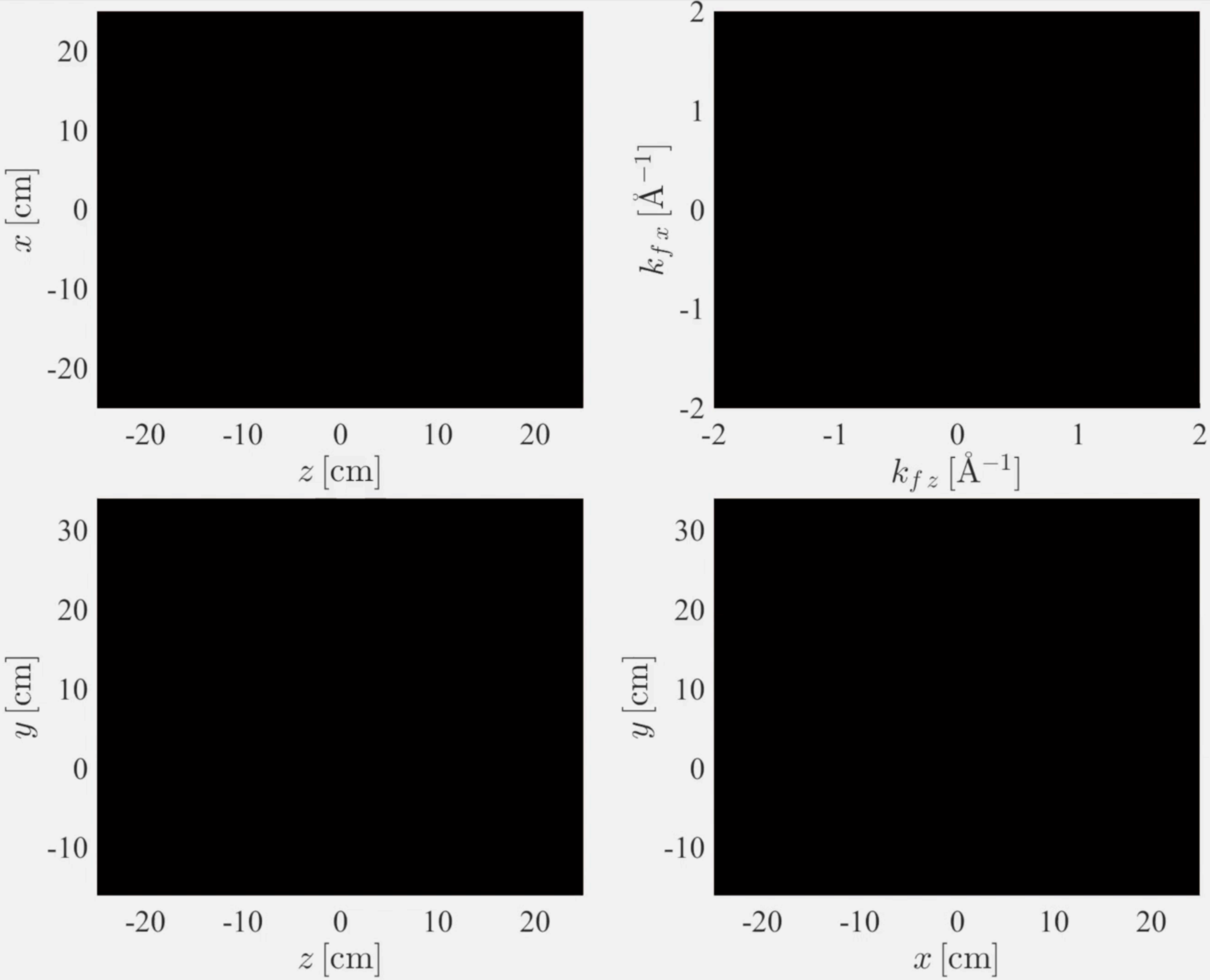






x [cm]
20
10
0
-10
-20
-20 -10 0 10 20
z [cm]
k_{fx} [Å^{-1}]
2
1
0
-1
-2
-2 -1 0 1 2
k_{fz} [Å^{-1}]
y [cm]
30
20
10
0
-10
-20 -10 0 10 20
z [cm]
y [cm]
30
20
10
0
-10
-20 -10 0 10 20
x [cm]

MACS Instrument simulation

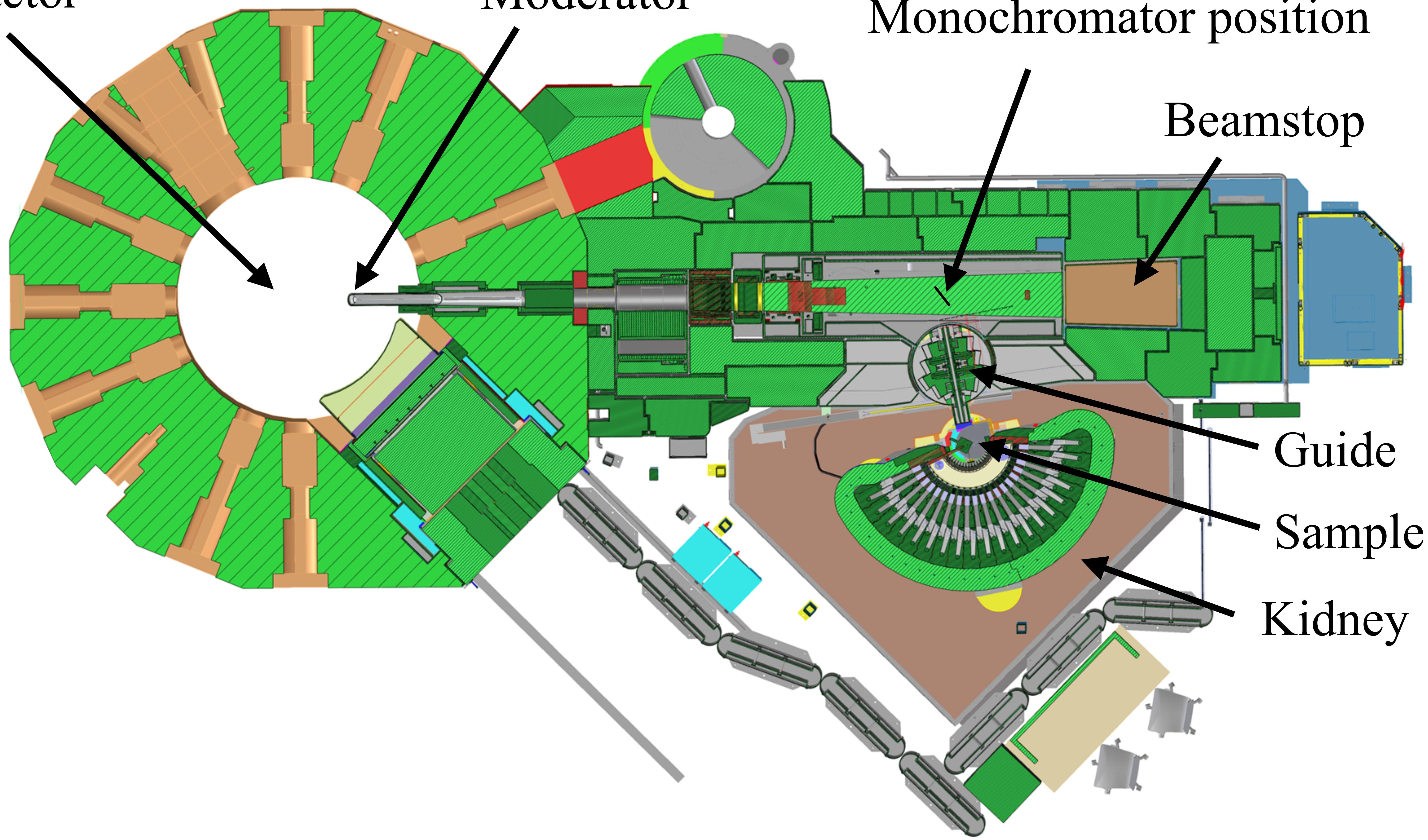
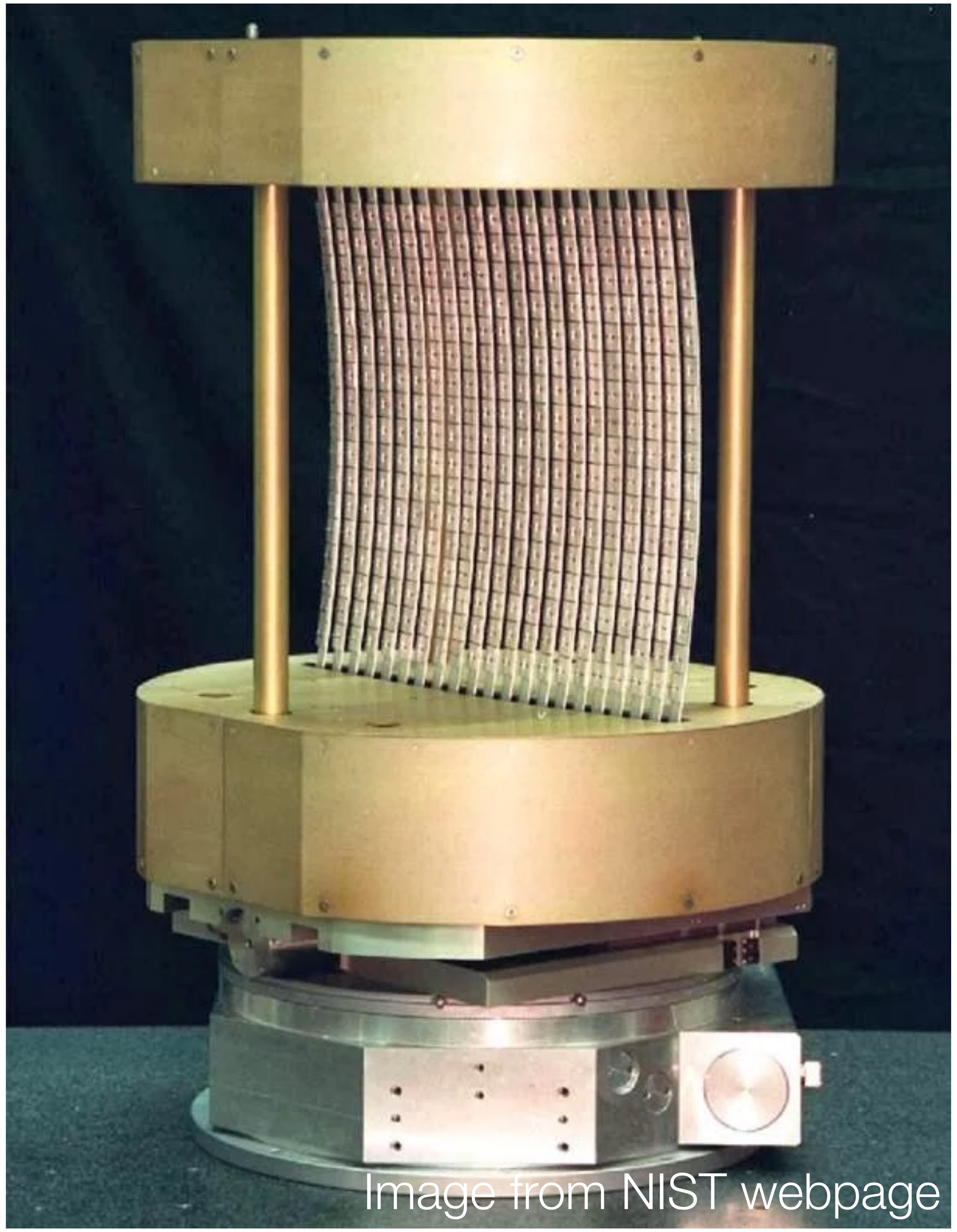
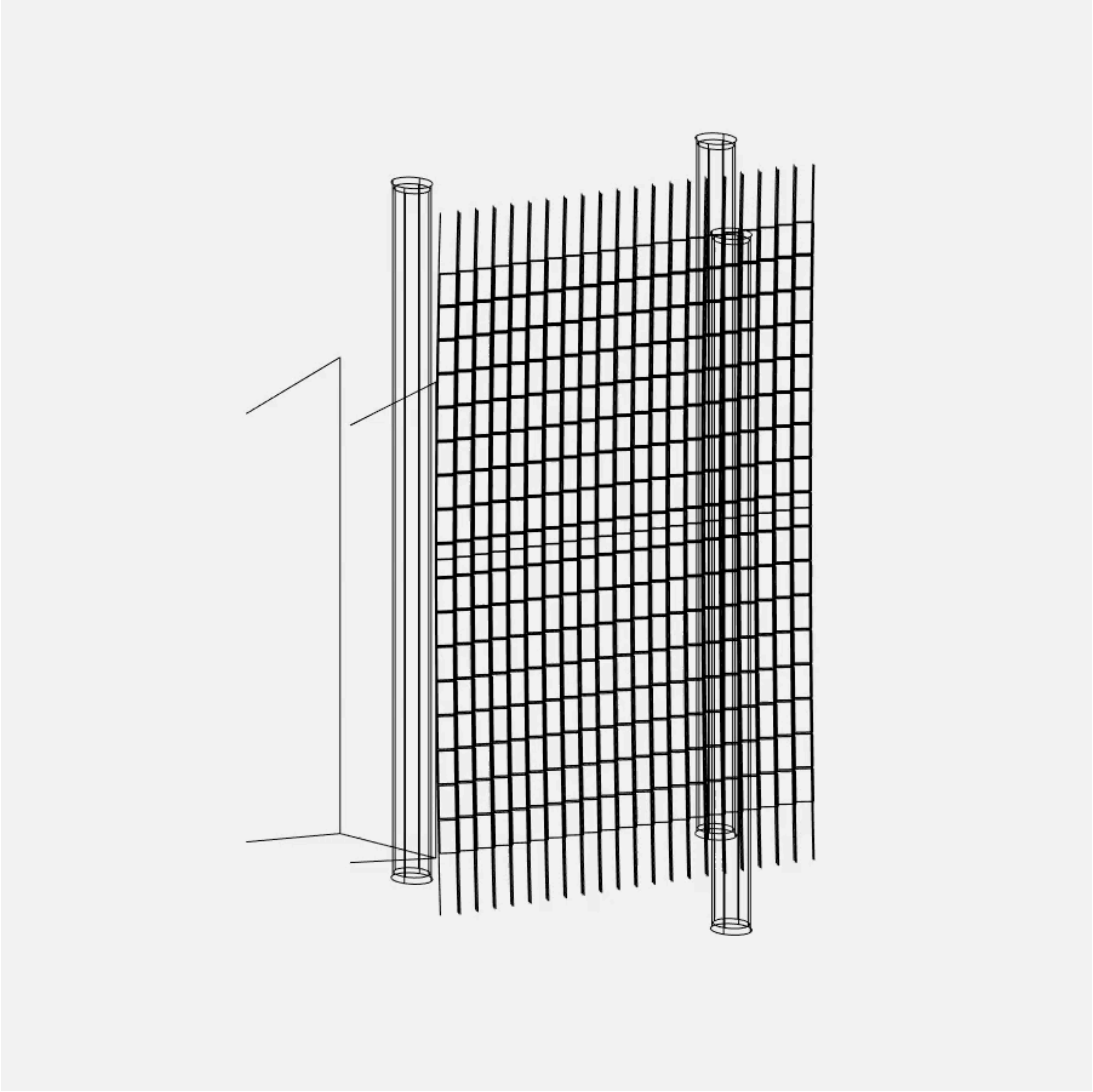
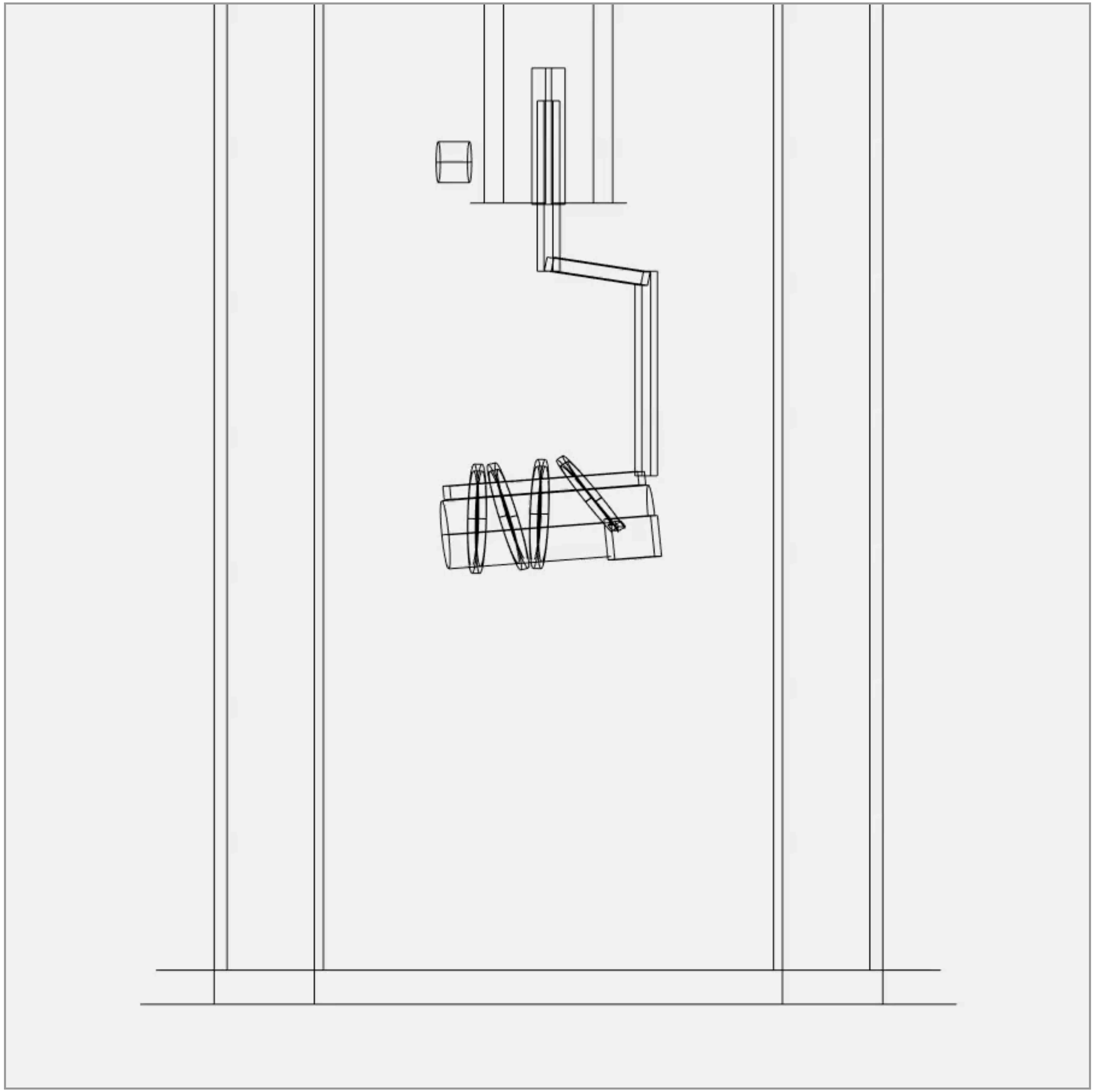


Image from NIST webpage

MACS Instrument simulation

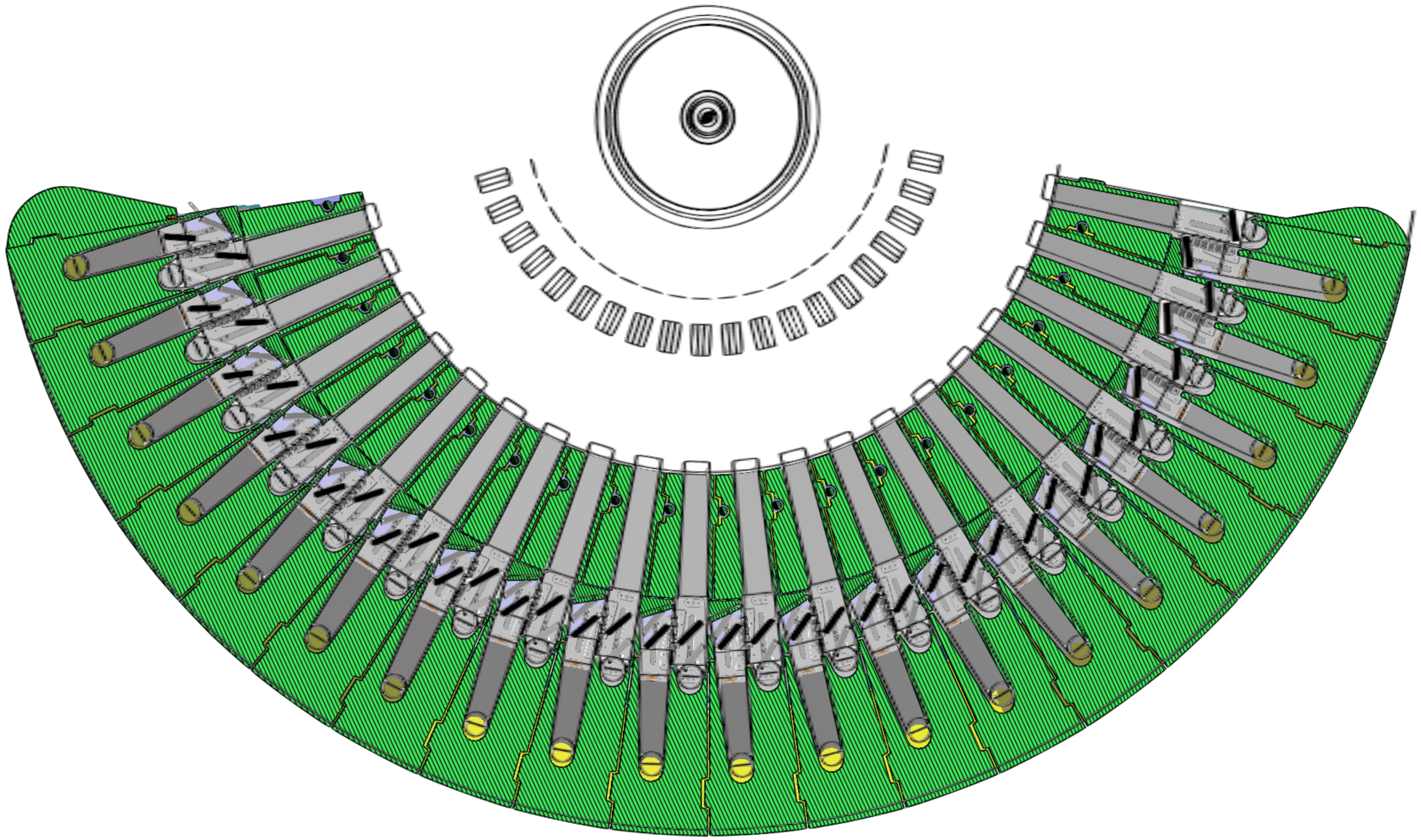






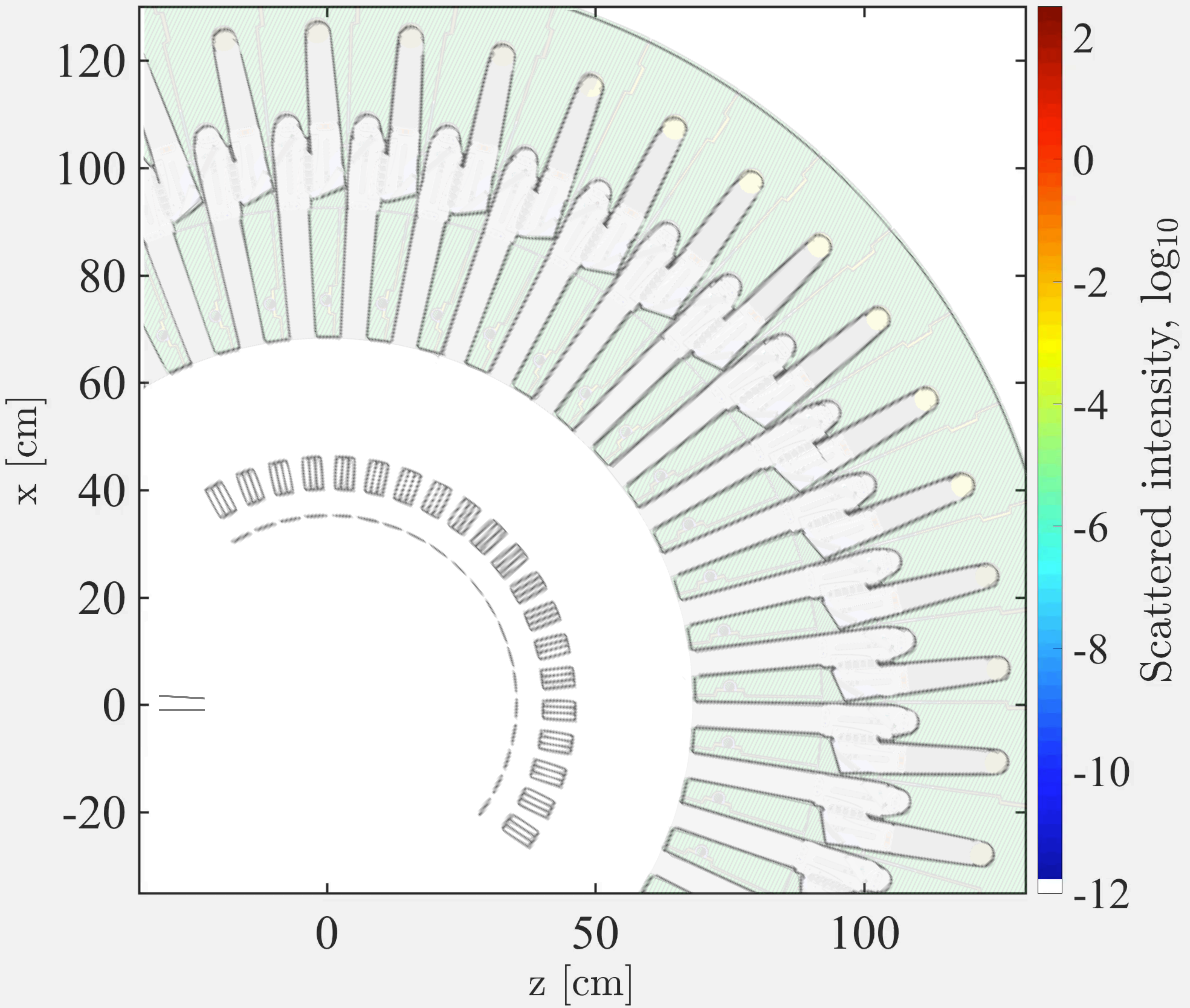
MACS Instrument simulation

- CAD model of instrument backend
- More than 600 geometries
- 2 Union_master components



MACS

- Air scattering around cryostat
- Initial and final energy: 5 meV



MACS

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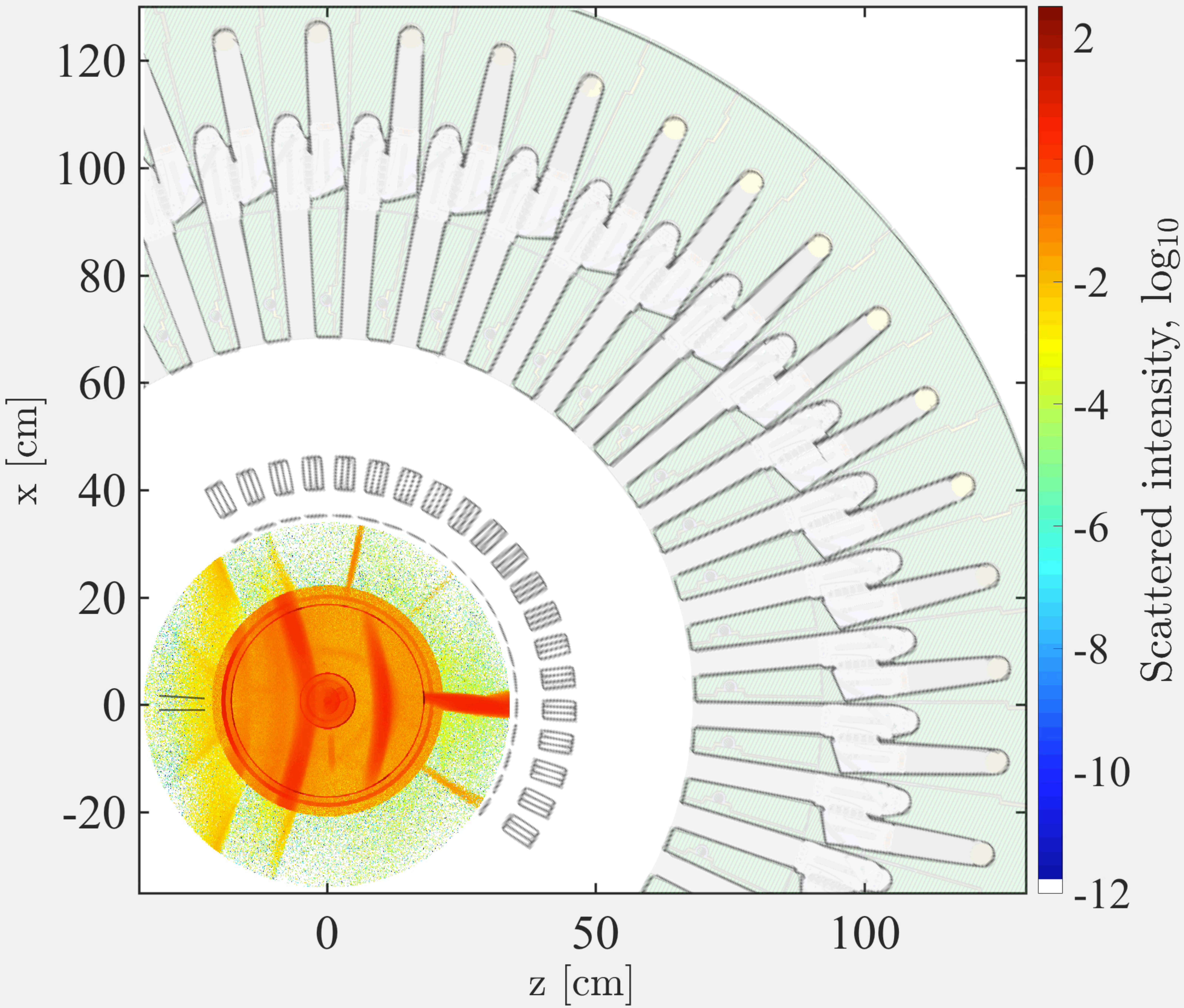
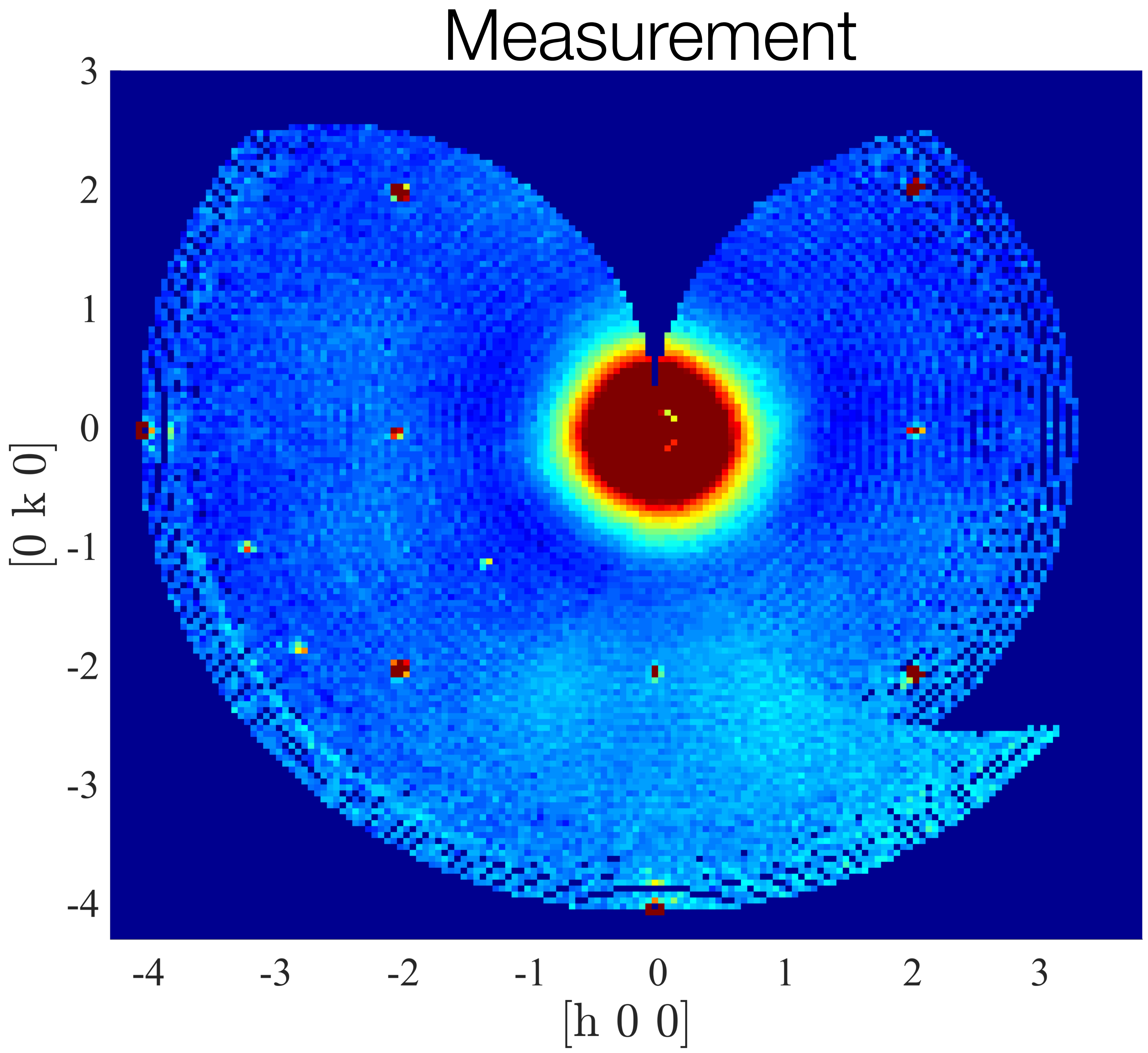
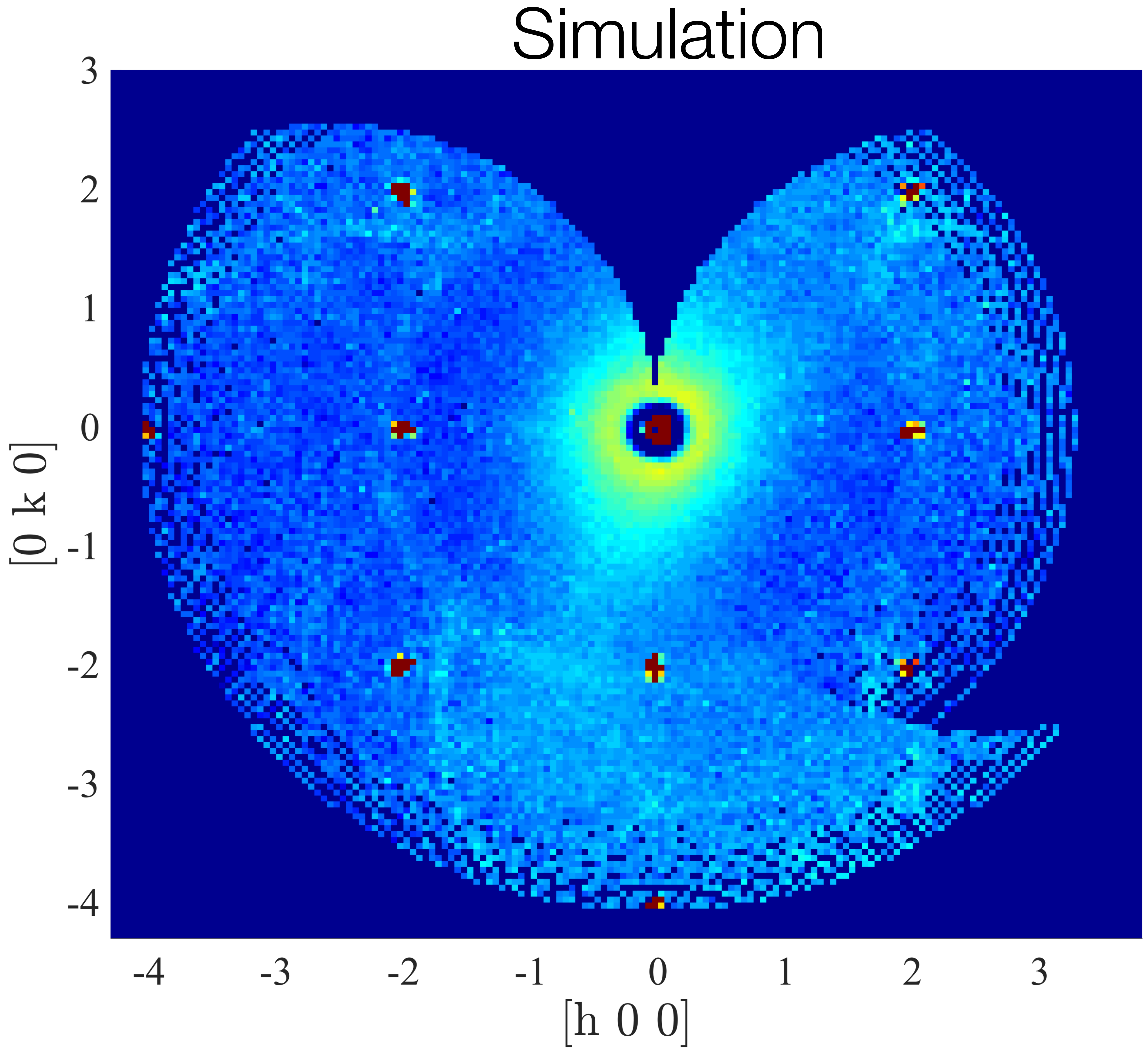


MACS Results





Conclusions on Union components

- In McStas 2.4 under contrib/union
- Source code on github with McStas
- Manual available from me (should remember to upload it!)
- Expands McStas to simulate multiple scattering in complex geometries
- Strong tools included for understanding the simulation results

Thank you for your attention!

Mads Bertelsen
University of Copenhagen

Extra slides for questions

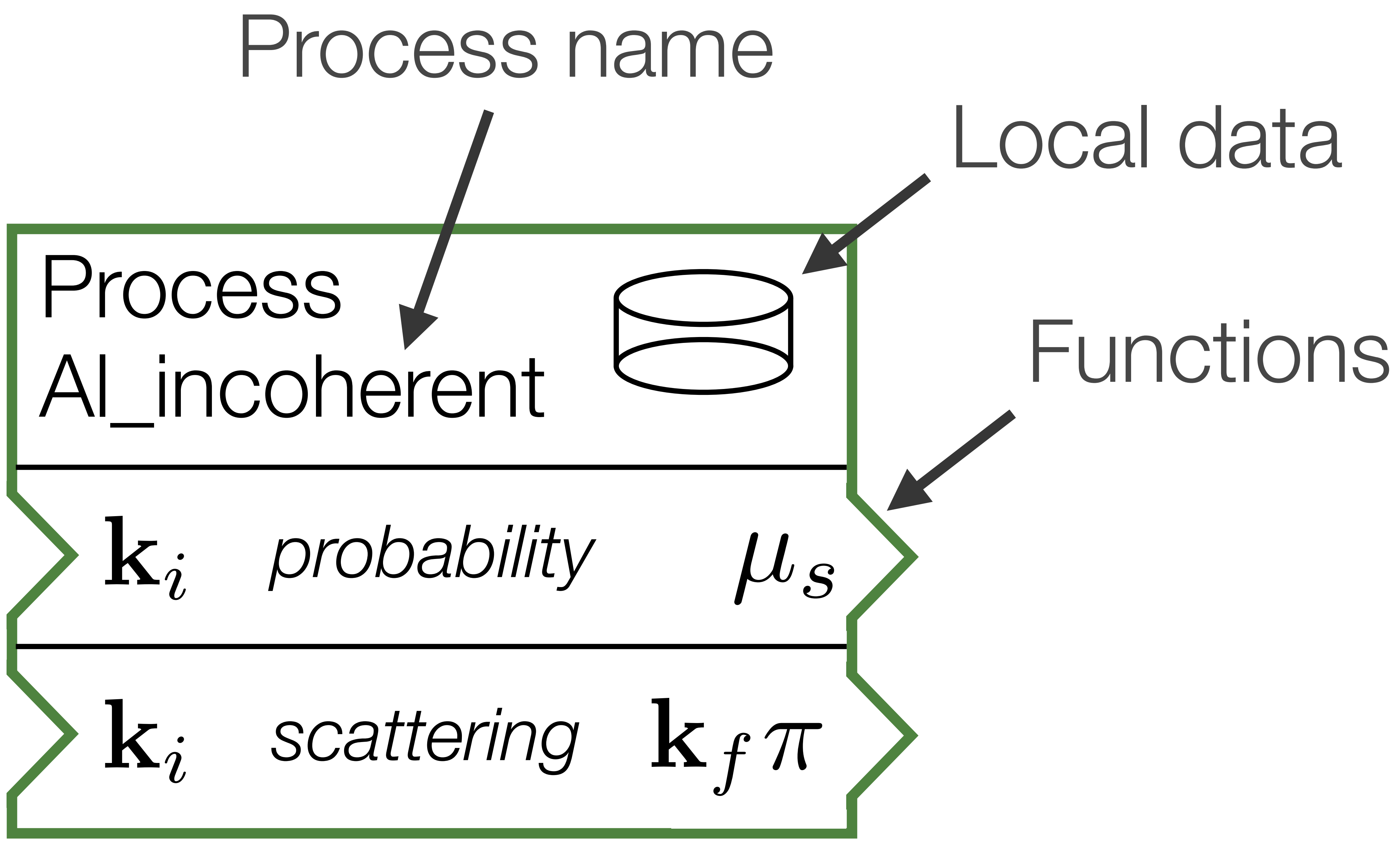
Mads Bertelsen
University of Copenhagen

MACS


x [cm]
100
50
0
0
50
100
z [cm]
2
0
-2
-4
-6
-8
-10
-12
Scattered intensity, $\log_{10}$
x component of k_f [Å^{-1}]
-2
-1
0
1
2
-2
-1
0
1
2
z component of k_f [Å^{-1}]
2
0
-2
-4
-6
-8
Scattered intensity, $\log_{10}$

McStas Union components - Physics

- Description of physics in Union
- Process McStas components
- Easy to contribute



Beam attenuation $I/I_0 = e^{-\mu z}$

Inverse penetration depth $\mu_{tot} = \mu_{abs} + \mu_s$

Weight factor manipulation $P = f\pi$

McStas Union components - Physics

- Materials collect a number of processes
- Includes absorption description

Total scattering $\mu_s = \sum_i^N \mu_i$

Total $\mu_{tot} = \mu_{abs} + \mu_s$

Weight correction for absorption

$$\pi = P_{scat}/f_s = \mu_s/\mu_{total}$$

Probability for process *i* $p_i = \frac{\mu_i}{\mu_s}$