McStas and McStasScript

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European Spallation Source

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McStas - Overview

- Name: Monte Carlo Simulation of Triple Axis Spectrometer
- Now simulates all kinds of neutron scattering instrumentation
- From neutron source to detector

- Core developers at DTU / ESS
- Open source community project, many contributions

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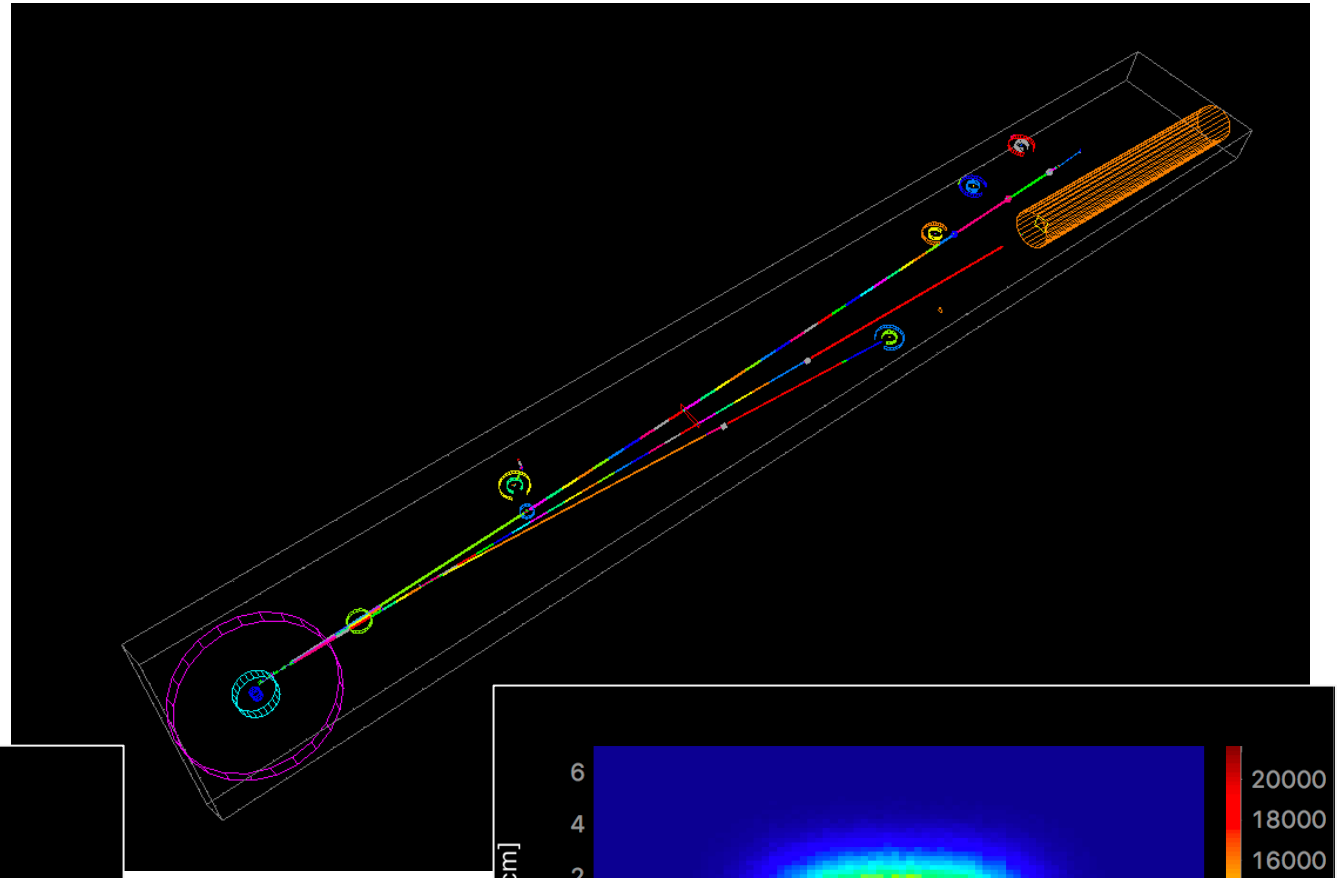
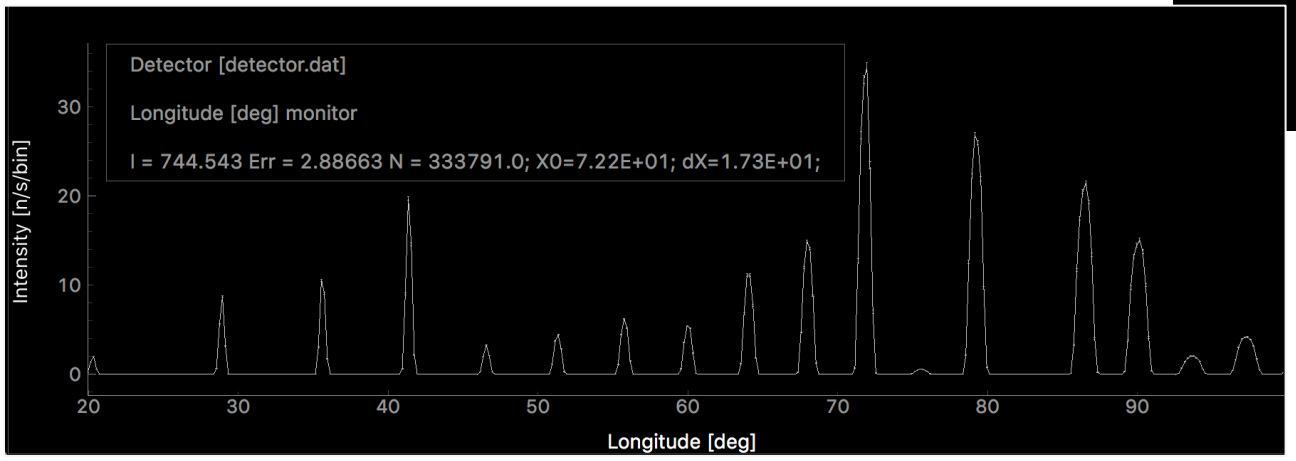
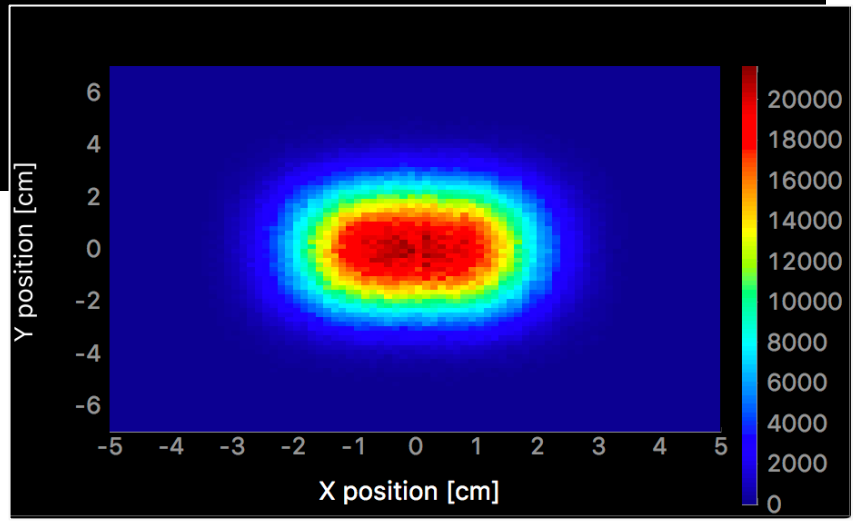
McStas - Overview

- 3D model and physics
- Construct instrument from pool of components
- Each component describe spatially separate part of the instrument







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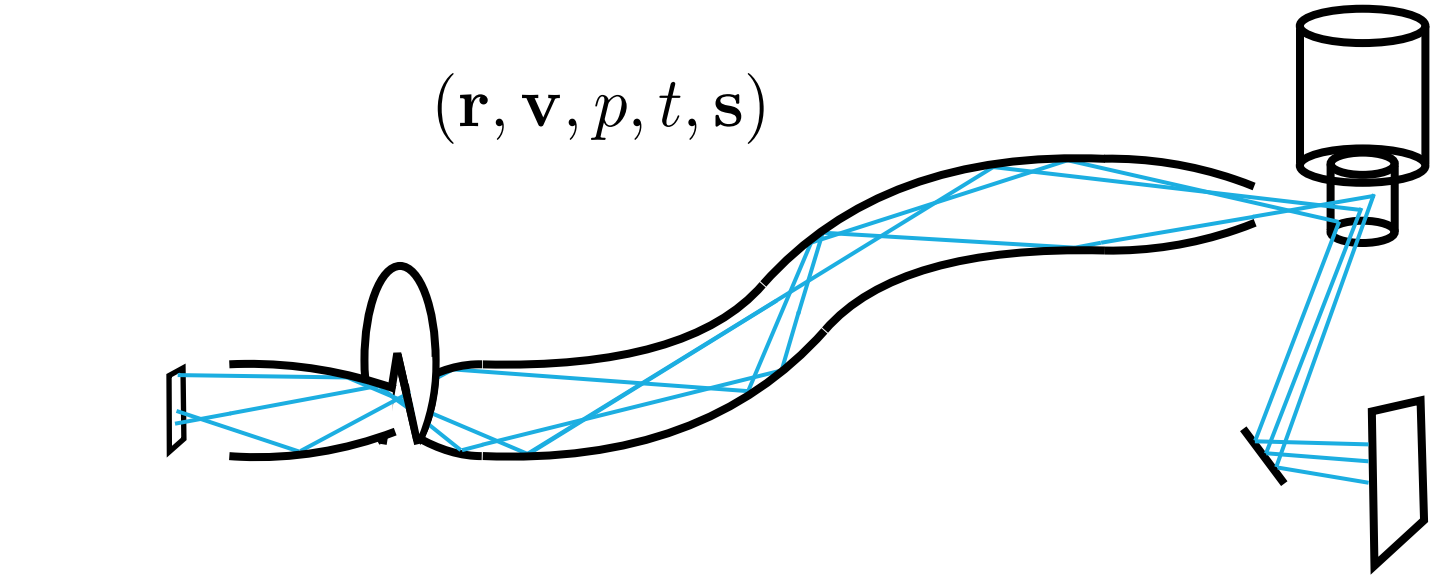
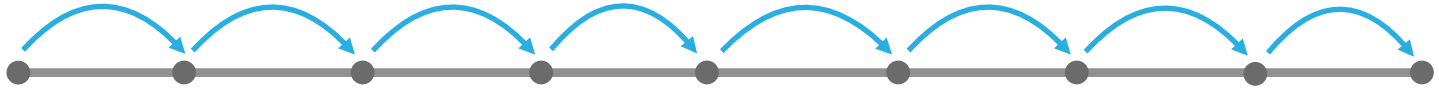
McStas - Components

- **Sources**
  - From file
  - Analytical
- **Optics**
  - Guides
  - Choppers
  - Monochromator
- **Sample**
  - Crystaline
  - Inelastic
  - Large scale structures
- **Monitors**





Sequence of components

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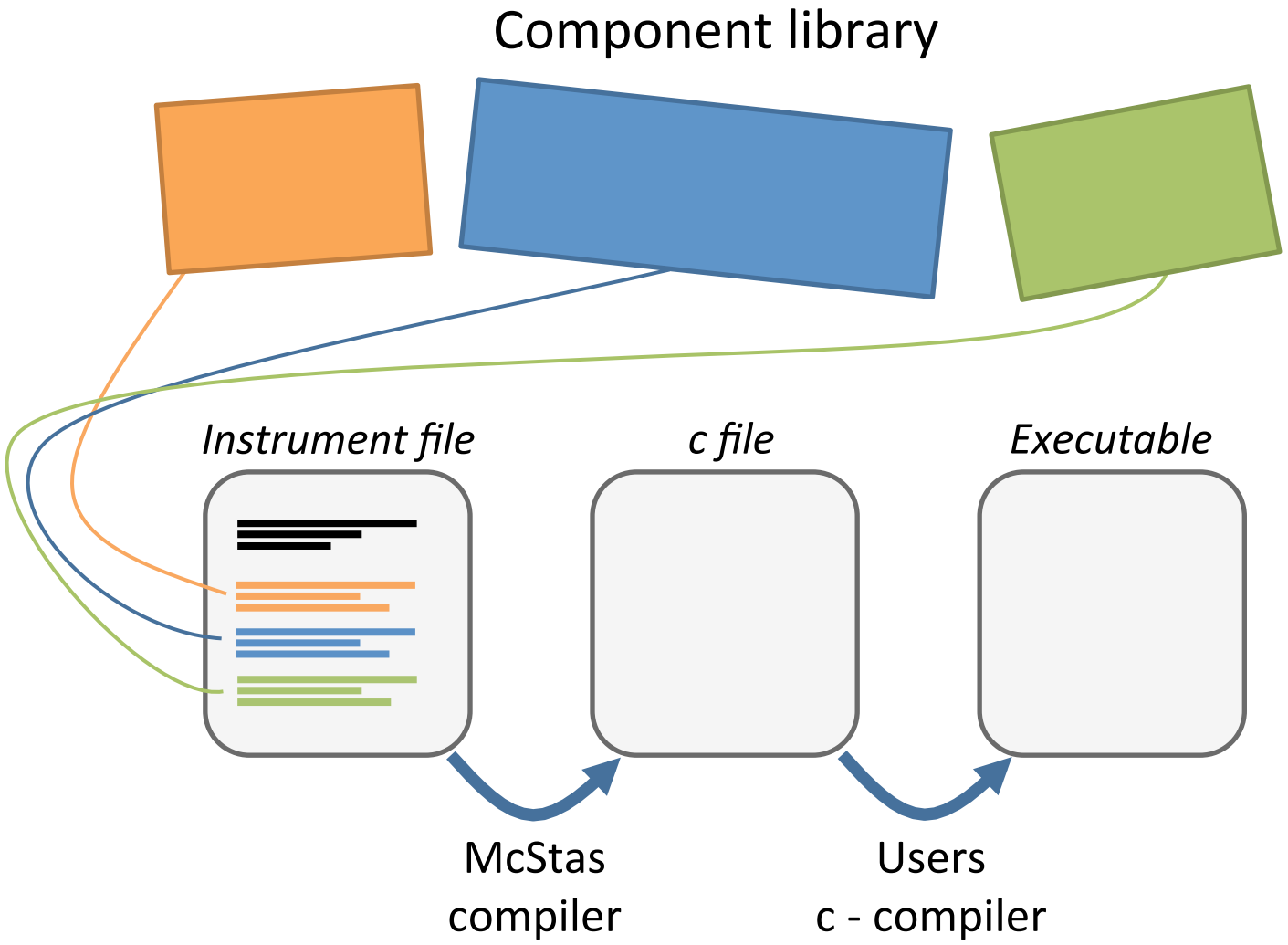
McStas – Technical

- **Instrument file (meta language)**
  1. Instrument definition
  2. Declare section
  3. Initialize section
  4. Trace section
  5. Finally section

- **Instrument to data with one utility**
  - mcrun on command line
  - mcgui graphical user interface



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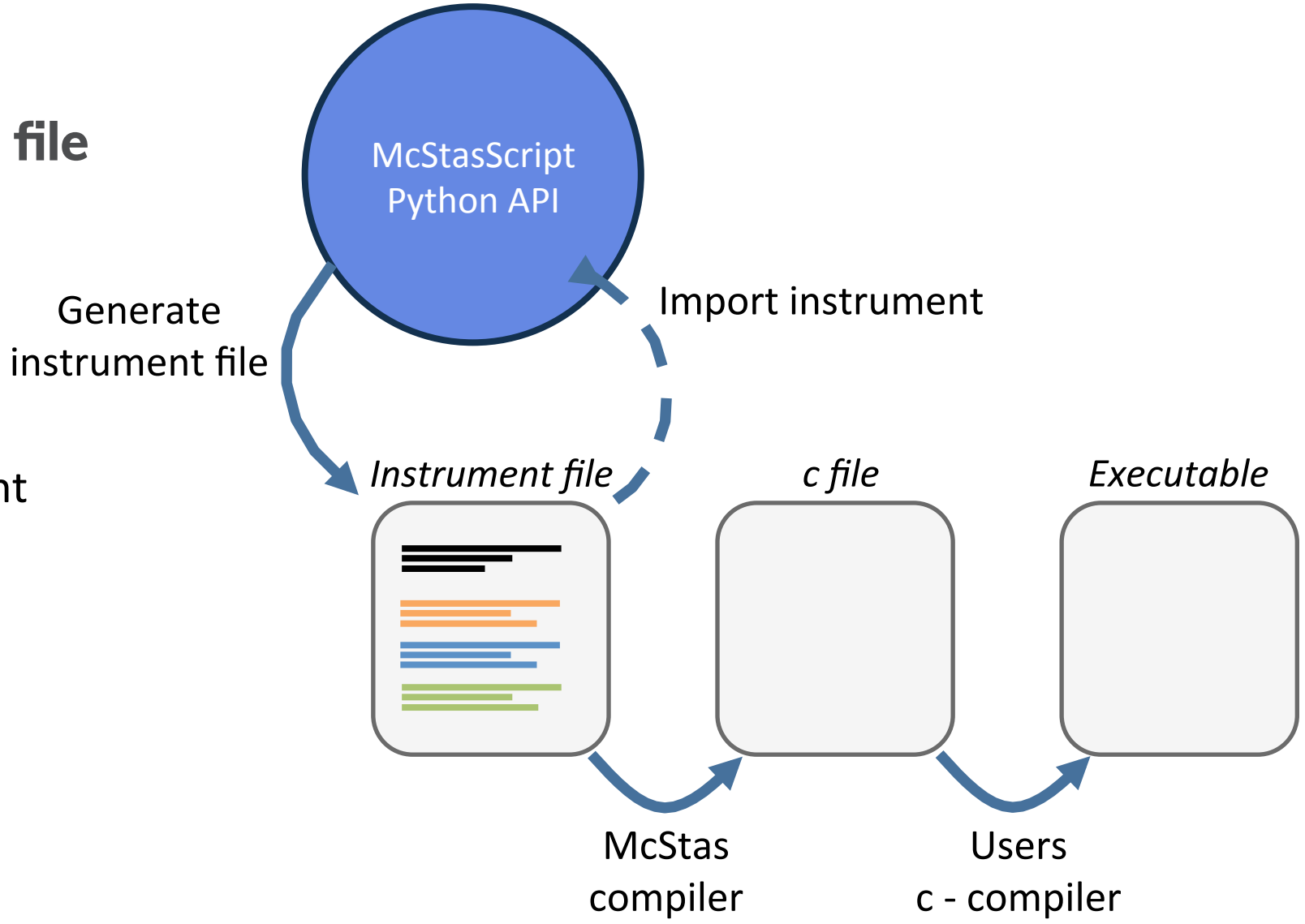
McStasScript

- **Generate instrument file from python API**
- **Advantages:**
  - for loops
  - Functions
  - Flexible code placement



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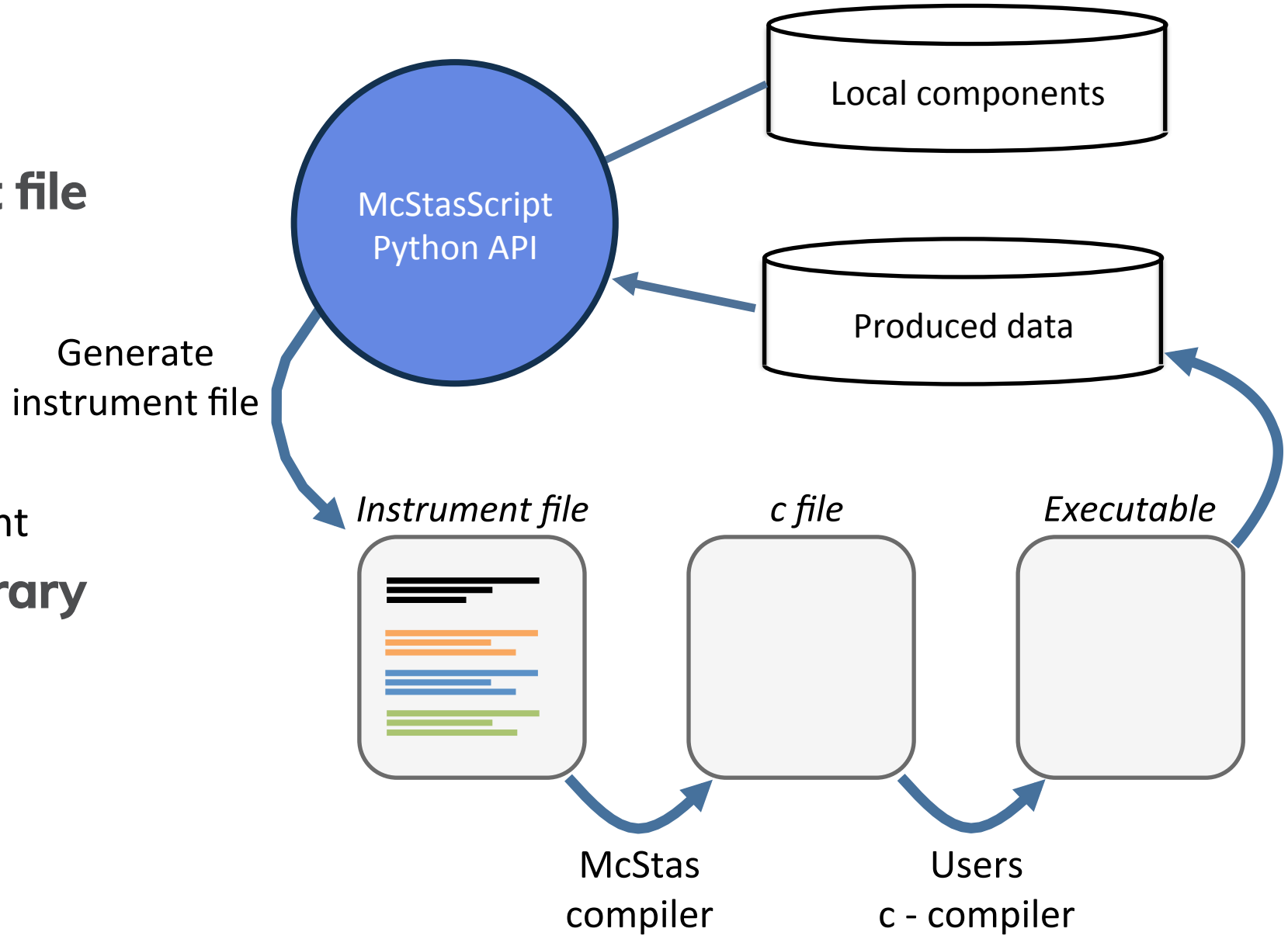
McStasScript

- **Generate instrument file from python API**
- **Advantages:**
  - for loops
  - Functions
  - Flexible code placement
- **Read component library**
- **Execute simulation**
- **Load data**



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McStasScript

- **Installation**

  Python –m pip install McStasScript

- **Configuration**
  - Set path to mcrun utility
  - Set path to components

```
In [2]: from mcstasscript.interface import instr, plotter, functions
```

```
In [3]: my_config = functions.Configurator()
        my_config.set_line_length(72)
        my_config.set_mcrun_path("/Applications/McStas-2.5.app/Contents/Resources/mcstas/2.5/bin/")
        my_config.set_mcstas_path("/Applications/McStas-2.5.app/Contents/Resources/mcstas/2.5/")
```

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McStasScript

- Create a new instrument object

```
In [3]: demo = instr.McStas_instr("presentation_demo")
```

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McStasScript

- Add instrument parameter
- Add a component
- Print component state

```
In [4]: demo.add_parameter("wavelength", value=4.0, comment="[AA] Wavelength simulated")
        demo.show_parameters()
```

```
wavelength  =  4.0  // [AA] Wavelength simulated
```

```
In [5]: src = demo.add_component("source", "Source_simple")
        src.xwidth = 0.11
        src.yheight = 0.11
        src.focus_xw = 0.05
        src.focus_yh = 0.05
        src.dist = 2.0
        src.lambda0 = "wavelength"
        src.dlambda = "0.1*wavelength"
        src.flux = 1E13
```

```
In [6]: src.print_long()
```

```
COMPONENT source = Source_simple
  yheight = 0.11 [m]
  xwidth = 0.11 [m]
  dist = 2.0 [m]
  focus_xw = 0.05 [m]
  focus_yh = 0.05 [m]
  lambda0 = wavelength [AA]
  dlambda = 0.1*wavelength [AA]
  flux = 10000000000000.0 [1/(s*cm**2*st*energy unit)]
AT [0, 0, 0] ABSOLUTE
```

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McStasScript

- **Include code in the simulation, declare and initialize**

```
In [7]: monochromator_Q = 1.8734
        demo.add_declare_var("double", "mono_Q", value=monochromator_Q)
        demo.add_declare_var("double", "wavevector")
        demo.append_initialize("wavevector = 2*PI/wavelength;")

        demo.add_declare_var("double", "mono_rotation")
        demo.append_initialize("mono_rotation = asin(mono_Q/(2.0*wavevector))*RAD2DEG;")
```

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McStasScript

- Include code in the simulation, declare and initialize
- Use in component

```
In [7]: monochromator_Q = 1.8734
        demo.add_declare_var("double", "mono_Q", value=monochromator_Q)
        demo.add_declare_var("double", "wavevector")
        demo.append_initialize("wavevector = 2*PI/wavelength;")

        demo.add_declare_var("double", "mono_rotation")
        demo.append_initialize("mono_rotation = asin(mono_Q/(2.0*wavevector))*RAD2DEG;")

In [8]: mono = demo.add_component("mono", "Monochromator_flat")

In [9]: mono.zwidth = 0.05
        mono.yheight = 0.05
        mono.Q = monochromator_Q
        mono.set_AT([0, 0, 2], RELATIVE="source")
        mono.set_ROTATED([0, "mono_rotation", 0], RELATIVE="source")
```

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McStasScript

- Add a monitor to collect data

In [10]:
```
beam_direction = demo.add_component("beam_dir", "Arm", AT_RELATIVE="mono")
beam_direction.set_ROTATED([0, "mono_rotation", 0], RELATIVE="mono")

detector = demo.add_component("detector", "PSD_monitor")
detector.xwidth = 0.1
detector.yheight = 0.1
detector.filename = "\"data.dat\""
detector.nx = 100
detector.ny = 100
detector.set_AT([0,0,2], RELATIVE="beam_dir")
```

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McStasScript

- Run the simulation from python
- Data returned as simple object with numpy data arrays

```
In [16]: data = demo.run_full_instrument(ncount=1E7, foldername="demo", increment_folder_name=True,
                                         parameters={"wavelength" : 3.5})
```

```
INFO: Using directory: "demo_0"
INFO: Regenerating c-file: presentation_demo.c
CFLAGS=
INFO: Recompiling: ./presentation_demo.out
INFO: ===
INFO: Placing instr file copy presentation_demo.instr in dataset demo_0

Detector: detector_I=8.35572e+09 detector_ERR=2.10199e+07 detector_N=158020 "data.dat"
```

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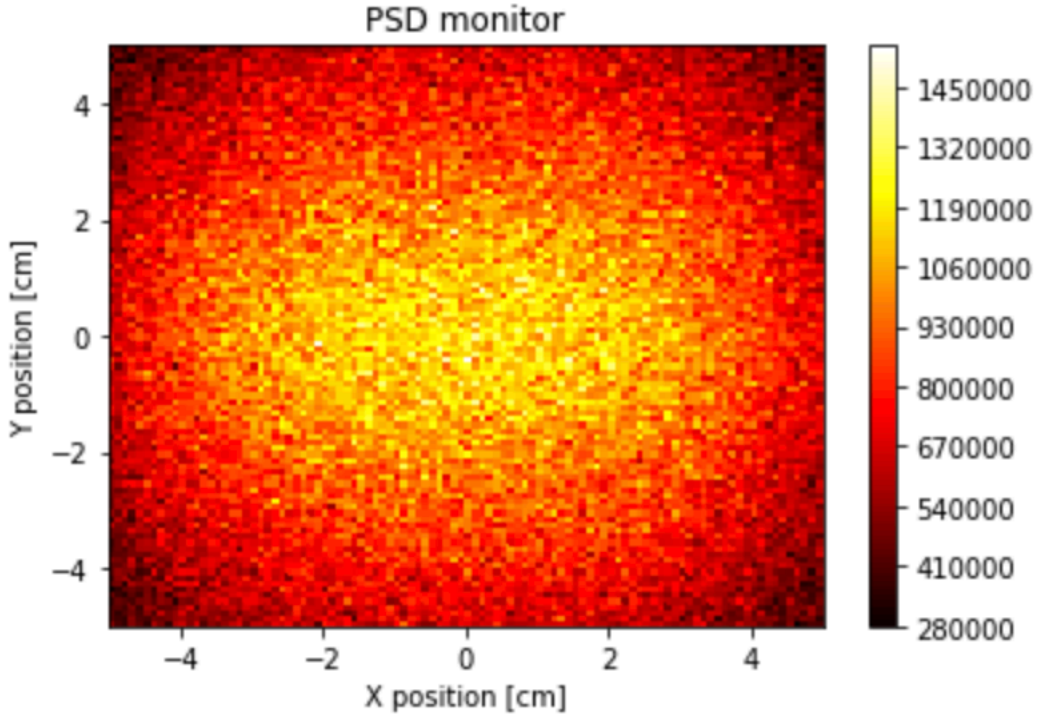
McStasScript

```
In [12]: plotter.make_plot(data)
```

```
number of elements in data list = 1
Plotting data with name detector
```



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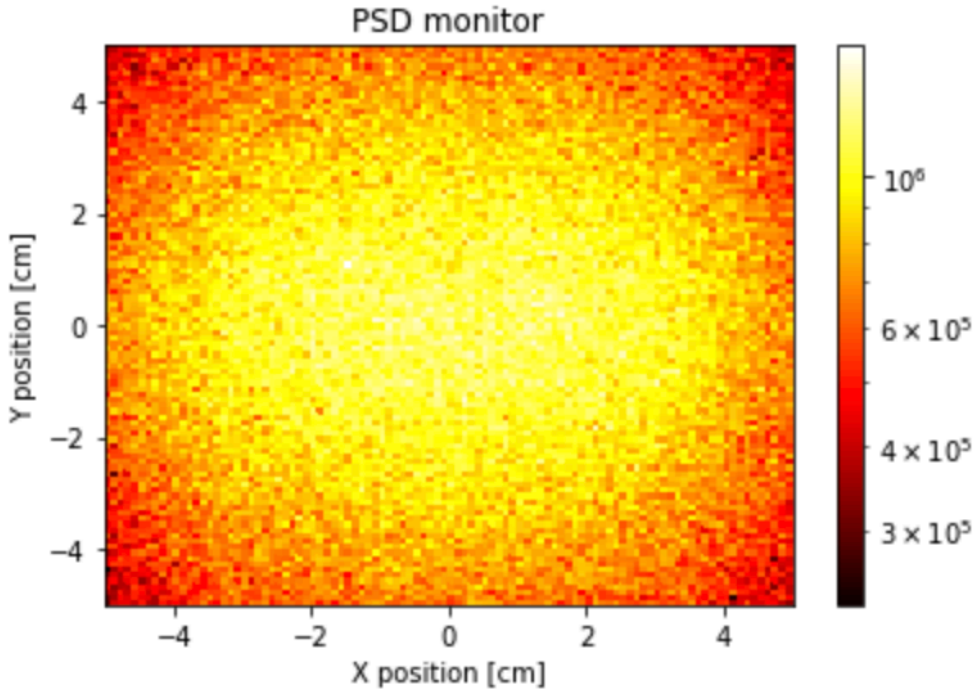
McStasScript

```
In [13]: functions.name_plot_options("detector", data, log=True)

In [14]: plotter.make_plot(data)
```

```
number of elements in data list = 1
Plotting data with name detector
```



Plot preferences included in data object

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McStasScript

In [1]:
```
from mcstasscript.interface import instr, plotter, functions, reader
```

In [2]:
```
InstrReader = reader.McStas_file("presentation_demo.instr")
```

In [3]:
```
InstrReader.write_python_file("generated_presentation.py", force=True)
```

In [4]:
```
demo = instr.McStas_instr("generated_presentation_demo")
InstrReader.add_to_instr(demo)
```

In [5]:
```
demo.print_components()
```

```
source    Source_simple       AT      (0, 0, 0)              ABSOLUTE
                              ROTATED (0, 0, 0)              ABSOLUTE
mono      Monochromator_flat  AT      (0, 0, 2)              RELATIVE source
                              ROTATED (0, mono_rotation, 0)  RELATIVE source
beam_dir  Arm                 AT      (0, 0, 0)              RELATIVE mono
                              ROTATED (0, mono_rotation, 0)  RELATIVE mono
detector  PSD_monitor         AT      (0, 0, 2)              RELATIVE beam_dir
                              ROTATED (0, 0, 0)              RELATIVE beam_dir
```

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McStasScript

- Python API as an alternative to standard McStas workflow
- Still work to do on API, may rename some methods / functions / keywords
- Improvements on plotting and data handling
- Review pending from co-workers
- Continous integration will be set up

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PaNOSC WP5 deliverables

- **openPMD**
  - Has been postponed slightly in favor of building an API
  - Have example dataset and extension document
  - Need to make McStas in/out components
- **Documented API**
  - Have an API, will need further improvements
  - Both docstrings and pdf documentation
  - 199 unit tests of core functionallity, lacks test of plotting / instrument reader
  - Wish to add continous integration
- **Release of examples in Jupyter Notebook**
  - Can generate python scripts for McStas instruments (Hundreds available)
  - Can create more examples that emphesises python advantages

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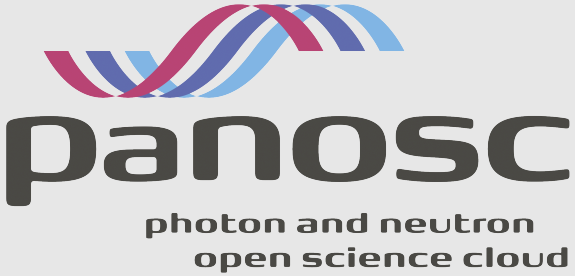

Thank you

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