

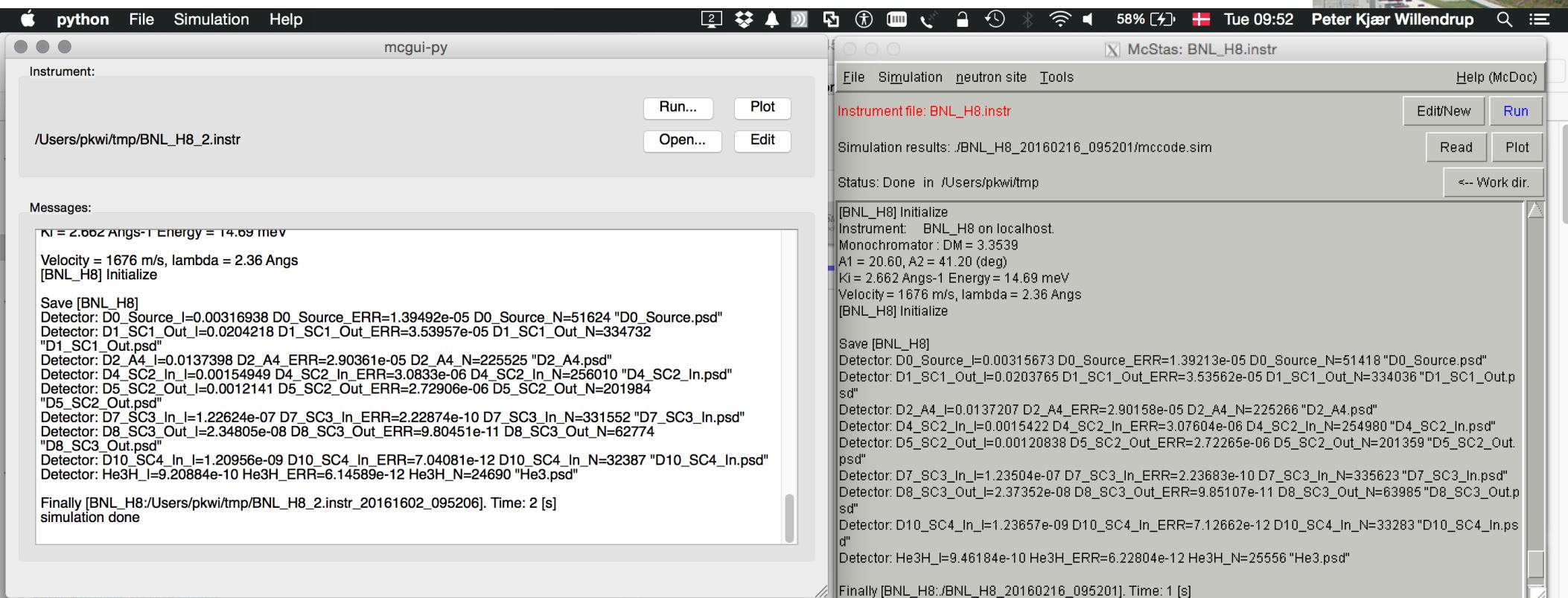
ORNL McStas workshop Thursday morning



An overview of the McStas tools

Presenter: Peter Willendrup

mcgui - pl vs py versions



Instrument: /Users/pkwi/tmp/BNL_H8_2.instr

Run... Plot
Open... Edit

Messages:

```
KI = 2.002 Angs-1 Energy = 14.69 meV
Velocity = 1676 m/s, lambda = 2.36 Angs
[BNL_H8] Initialize

Save [BNL_H8]
Detector: D0_Source_I=0.00316938 D0_Source_ERR=1.39492e-05 D0_Source_N=51624 "D0_Source.psd"
Detector: D1_SC1_Out_I=0.0204218 D1_SC1_Out_ERR=3.53957e-05 D1_SC1_Out_N=334732
"D1_SC1_Out.psd"
Detector: D2_A4_I=0.0137398 D2_A4_ERR=2.90361e-05 D2_A4_N=225525 "D2_A4.psd"
Detector: D4_SC2_In_I=0.00154949 D4_SC2_In_ERR=3.0833e-06 D4_SC2_In_N=256010 "D4_SC2_In.psd"
Detector: D5_SC2_Out_I=0.0012141 D5_SC2_Out_ERR=2.72906e-06 D5_SC2_Out_N=201984
"D5_SC2_Out.psd"
Detector: D7_SC3_In_I=1.22624e-07 D7_SC3_In_ERR=2.22874e-10 D7_SC3_In_N=331552 "D7_SC3_In.psd"
Detector: D8_SC3_Out_I=2.34805e-08 D8_SC3_Out_ERR=9.80451e-11 D8_SC3_Out_N=62774
"D8_SC3_Out.psd"
Detector: D10_SC4_In_I=1.20956e-09 D10_SC4_In_ERR=7.04081e-12 D10_SC4_In_N=32387 "D10_SC4_In.psd"
Detector: He3H_I=9.20884e-10 He3H_ERR=6.14589e-12 He3H_N=24690 "He3.psd"

Finally [BNL_H8:/Users/pkwi/tmp/BNL_H8_2.instr_20161602_095206]. Time: 2 [s]
simulation done
```

Instrument file: BNL_H8.instr

File Simulation neutron site Tools Help (McDoc)

Simulation results: ./BNL_H8_20160216_095201/mccode.sim

Status: Done in /Users/pkwi/tmp

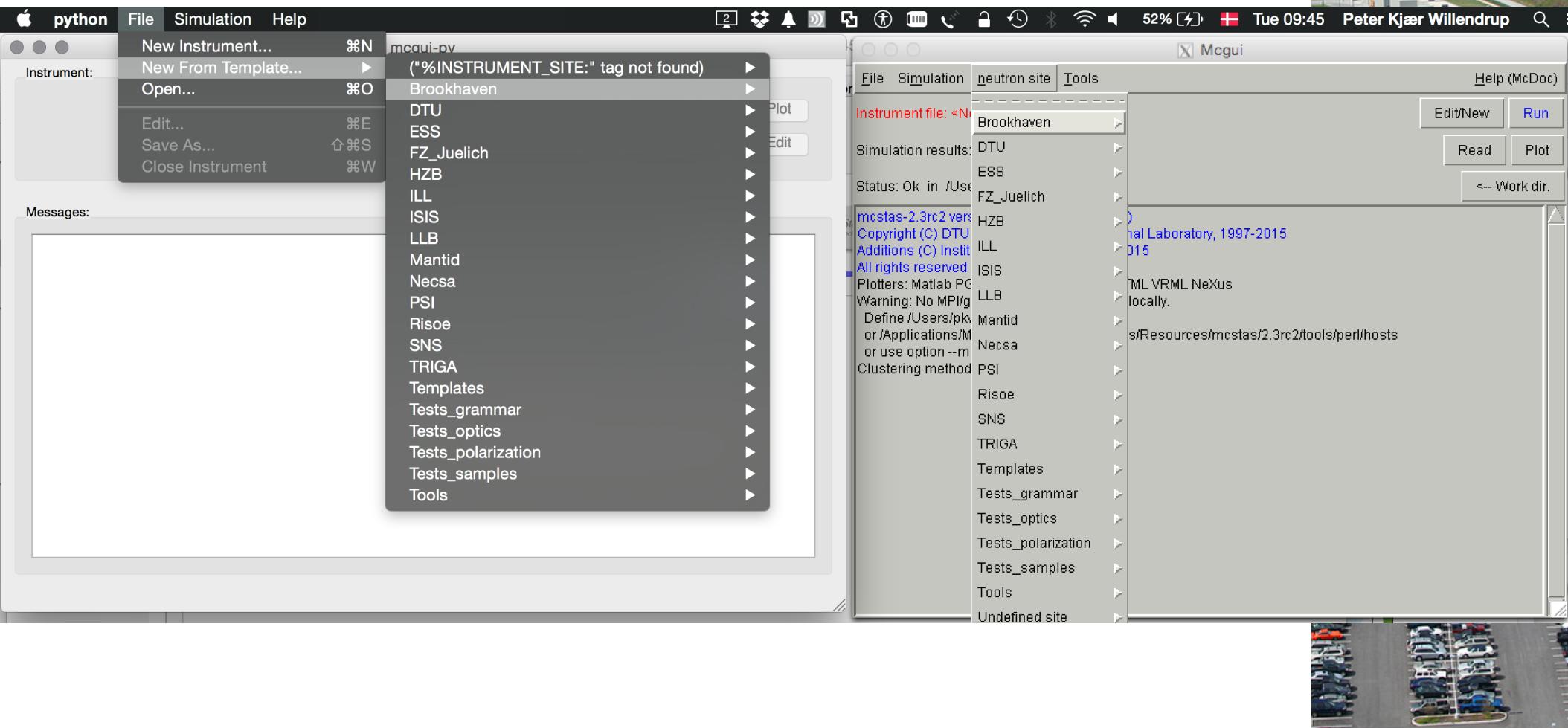
[BNL_H8] Initialize
 Instrument: BNL_H8 on localhost.
 Monochromator : DM = 3.3539
 A1 = 20.60, A2 = 41.20 (deg)
 KI = 2.662 Angs-1 Energy = 14.69 meV
 Velocity = 1676 m/s, lambda = 2.36 Angs
[BNL_H8] Initialize

Save [BNL_H8]
Detector: D0_Source_I=0.00315673 D0_Source_ERR=1.39213e-05 D0_Source_N=51418 "D0_Source.psd"
Detector: D1_SC1_Out_I=0.0203765 D1_SC1_Out_ERR=3.53562e-05 D1_SC1_Out_N=334036 "D1_SC1_Out.psd"
Detector: D2_A4_I=0.0137207 D2_A4_ERR=2.90158e-05 D2_A4_N=225266 "D2_A4.psd"
Detector: D4_SC2_In_I=0.0015422 D4_SC2_In_ERR=3.07604e-06 D4_SC2_In_N=254980 "D4_SC2_In.psd"
Detector: D5_SC2_Out_I=0.00120838 D5_SC2_Out_ERR=2.72265e-06 D5_SC2_Out_N=201359 "D5_SC2_Out.psd"
Detector: D7_SC3_In_I=1.23504e-07 D7_SC3_In_ERR=2.23683e-10 D7_SC3_In_N=335623 "D7_SC3_In.psd"
Detector: D8_SC3_Out_I=2.37352e-08 D8_SC3_Out_ERR=9.85107e-11 D8_SC3_Out_N=63985 "D8_SC3_Out.psd"
Detector: D10_SC4_In_I=1.23657e-09 D10_SC4_In_ERR=7.12662e-12 D10_SC4_In_N=33283 "D10_SC4_In.psd"
Detector: He3H_I=9.46184e-10 He3H_ERR=6.22804e-12 He3H_N=25556 "He3.psd"

Finally [BNL_H8:/BNL_H8_20160216_095201]. Time: 1 [s]



mcgui (python) vs mcgui.pl/mogui-pl



*mcstas: /Users/pkwi/tmp/BNL_H8_2.instr

```
TRACE
/* Source description */
COMPONENT Origin=Progress_bar()
AT (0,0,0) ABSOLUTE

/* a flat constant source */
COMPONENT Source = Source_simple(
    radius = 0.10,
    dist = 2.7473,
    focus_xw = 0.031, focus_yh = 0.054,
    E0 = Ei,
    dE = 0.03*Ei)
AT (0,0,0) ABSOLUTE
```

```
CO
COMPONENT
COPY
CavitiesIn
CavitiesOut
Collimator_ROC
Collimator_linear
Collimator_radial
```

```
nx=20, ny=20, filename="D1_SC1_Out.psd")
AT (0, 0, 0.9145) RELATIVE SC1
```

```
COMPONENT As1 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 3.6998) RELATIVE Source
```

```
COMPONENT As2 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.0808) RELATIVE Source
```

```
COMPONENT As3 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.1189) RELATIVE Source
```

```
COMPONENT As4 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.4141) RELATIVE Source
```

```
COMPONENT D2_A4 = PSD_monitor(
    xwidth = 0.04450, yheight= 0.0635,
    nx=20, ny=20, filename="D2_A4.psd")
AT (0, 0, 0.0001) RELATIVE As4
```

```
COMPONENT Mono_Cradle = Arm()
AT (0, 0, 5.2746) RELATIVE Source ROTATED (0, A1, 0) RELATIVE Source
```

```
SPLIT COMPONENT PG1Xtal = Monochromator_flat(
    zwidth = 0.1, yheight = 0.08,
```

Edit: BNL_H8.instr

```
File Edit Search View Insert

TRACE
/* Source description */
COMPONENT Origin=Progress_bar()
AT (0,0,0) ABSOLUTE

/* a flat constant source */
COMPONENT Source = Source_simple(
    radius = 0.10,
    dist = 2.7473,
    focus_xw = 0.031, focus_yh = 0.054,
    E0 = Ei,
    dE = 0.03*Ei)
AT (0,0,0) ABSOLUTE

COMPONENT D0_Source = PSD_monitor(
    xwidth = 0.03, yheight= 0.054,
    nx=20, ny=20, filename="D0_Source.psd")
AT (0, 0, 0.0001) RELATIVE Source

/* SC1 collimator. 40=3 slots, 20=6 slots */

COMPONENT SC1 = Guide(
    w1 = 0.031, h1 = 0.054, l = 0.9144,
    R0 = 1.0, Qc=0.021, alpha=6, m=1, W=0.0003)
AT (0, 0, 2.7473) RELATIVE Source

COMPONENT D1_SC1_Out = PSD_monitor(
    xwidth = 0.03, yheight= 0.054,
    nx=20, ny=20, filename="D1_SC1_Out.psd")
AT (0, 0, 0.9145) RELATIVE SC1

COMPONENT As1 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 3.6998) RELATIVE Source

COMPONENT As2 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.0808) RELATIVE Source

COMPONENT As3 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.1189) RELATIVE Source

COMPONENT As4 = Slit(
    xwidth = 0.04450, yheight= 0.0635)
AT (0, 0, 4.4141) RELATIVE Source
```

Line: 1 of 248 total, Column: 0

mcgui (python) vs mcgui.pl/mcgui-pl

Component: DiskChopper

Written by: Peter Willendrup
Date: March 9 2006
Version: \$Revision\$
Origin: Risoe
Release: McStas 2.0
Based on Chopper (Philipp Bernhardt), Jitter and beamstop from work by Kaspar Hewitt Klenoe (jan 2006), adjustments by Rob Bewey (march 2006)

Models a disc chopper with nslit identical slits, which are symmetrically distributed on the disc. At time t=0, the centre of the first slit opening will be situated at the vertical axis when phase=0.

For more complicated geometries, see component manual example of DiskChopper GROUPing.

If the chopper is the 1st chopper of the instrument, it sets t time with phase
- Only relevant for when using continuous source modules.

Example: DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=1) First chopper
DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=0)

Component definition: DiskChopper

Based on Chopper (Philipp Bernhardt), Jitter and beamstop from work by Kaspar Hewitt Klenoe (jan 2006), adjustments by Rob Bewey (march 2006)

Author: Peter Willendrup
Origin: Risoe
Instance name:

DESCRIPTION: (read it and fill-in PARAMETERS section below)

Models a disc chopper with nslit identical slits, which are symmetrically distributed on the disc. At time t=0, the centre of the first slit opening will be situated at the vertical axis when phase=0.

For more complicated geometries, see component manual example of DiskChopper GROUPing.

If the chopper is the 1st chopper of the instrument, it sets t time with phase
- Only relevant for when using continuous source modules.

Example: DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=1) First chopper
DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=0)

PARAMETERS:

(optional parameters may be left blank, see DESCRIPTION section)
Character type parameters usually require quoting, e.g. filename="name"

theta_0: [deg] (OPTIONAL, default 0)
AT (, ,) RELATIVE
ROTATED (, ,) RELATIVE

Insert Cancel Ok Cancel

October 2018

mcgui (python) vs mcgui.pl/mcgui-pl



python

Component: DiskChopper

Written by: Peter Willendrup
Date: March 9 2006
Version: \$Revision\$
Origin: Risoe
Release: McStas 2.0
Based on Chopper (Philipp Bernhardt), Jitter and beamstop from work by Kaspar Hewitt Klenoe (jan 2006), adjustments by Rob Bewey (march 2006)

Models a disc chopper with nslit identical slits, which are symmetrically distributed on the disc. At time t=0, the centre of the first slit opening will be situated at the vertical axis when phase=0.

For more complicated geometries, see component manual example of DiskChopper GROUPing.

If the chopper is the 1st chopper of the instrument, it sets t time with phase
- Only relevant for when using continuous source modules.

Example: DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=1) First chopper
DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=0)

Component definition: DiskChopper
Based on Chopper (Philipp Bernhardt), Jitter and beamstop from work by Kaspar Hewitt Klenoe (jan 2006), adjustments by Rob Bewey (march 2006)

Written by: Peter Willendrup
Origin: Risoe
Name:
DESCRIPTION: (read it and fill-in PARAMETERS section below)

It's a disc chopper with nslit identical slits, which are symmetrically distributed on the disc. At time t=0, the centre of the first slit opening will be situated at the vertical axis when phase=0.

More complicated geometries, see component manual example of DiskChopper GROUPing.

The chopper is the 1st chopper of the instrument, it sets t time with phase
- Only relevant for when using continuous source modules.

Example: DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=1) First chopper
DiskChopper(radius=0.2, theta_0=10, nu=41.7, nslit=3, delay=0, isfirst=0)

PARAMETERS:
Optional parameters may be left blank, see DESCRIPTION section)
Character type parameters usually require quoting, e.g. filename="name"

theta_0: [deg] (OPTIONAL, default 0)
radius: (m) RELATIVE
yheight: (m) Slit height (if = 0, equal to radius). Auto centering of beam at half height.
nu: (Hz) Frequency of the Chopper, omega=2*Pi*nu (algebraic sign defines the direction of rotation)
nslit: (1) Number of slits, regularly arranged around the disk
jitter: (s) Jitter in the time phase
delay: (s) Time 'delay'.
isfirst: (0/1) Set it to 1 for the first chopper position in a cw source (it then spreads the neutron time distribution)
n_pulse: (1) Number of pulses (Only if isfirst)
abs_out: (0/1) Absorb neutrons hitting outside of chopper radius?

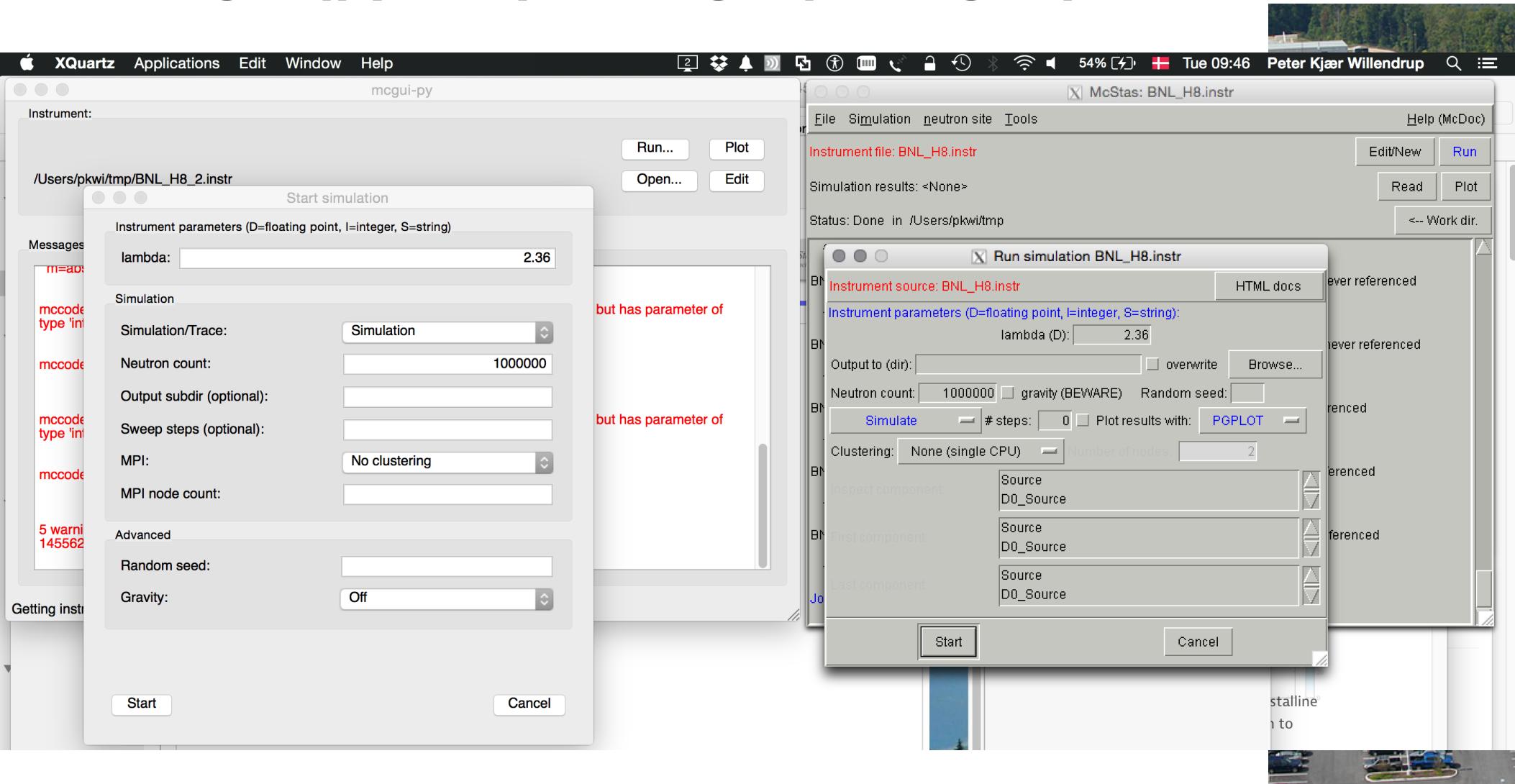
AT (, ,) RELATIVE PREVIOUS
ROTATED (, ,) RELATIVE PREVIOUS

Insert Cancel

AT (0, 0, 4.4141) RELATIVE Source

ROTATED (0, 0, 0) ABSOLUTE

mcgui (python) vs mcgui.pl/mcgui-pl



mcgui

mccode-py configuration

mcrun

mcrun-py

mcplot

mcplot

mcdisplay

mcdisplay-matplotlib-py

cc

gcc

C flags

-g -fopenmp -O2

MPIcc

mpicc

MPIrun

mpirun

nodes

4

Ok Save Cancel

Plotting options:

PGPLOT (original McStas)

3-pane view with PGPLOT trace

Clustering:

MPI (clusters)

Force compilation when gridding

Editor options:

Advanced built-in editor

GUI Palette

#c6c6c0

GUI Font

-*-arial-normal-r-*-*-120-*_*_*_*_*

Surround strings with quotes

Runtime tool options:

Execution/run command to use: mcrun

Plot command to use: mcplot

Trace command to use: mcdisplay

Compilation options:

Apply compiler flags: (define in textbox below)

-fopenmp -g -O2 -L/usr/local/lib -INeXus -DUSE_NEXUS

Compiler to use: cc

MPI Compiler to use: mpicc.ccc

MPIrun command to use: mpirun

Optimization options:

Precision 1e-3

OK



mcrun (py) vs. mcrun.pl/mcrun-pl version

```
XQuartzScreenSnapz004.png
tmp - pkwi@pkwi-mbp15: ~/tmp - bash - 88x50
pkwi@pkwi-mbp15:~/Pictures$ open XQuartzScreenSnapz00*
pkwi@pkwi-mbp15:~/Pictures$ cd
pkwi@pkwi-mbp15:~$ cd tmp/
pkwi@pkwi-mbp15:~/tmp$ mcrun-py --help
Usage: mcrun.py [-cpnN] Instr [-sndftgahil] params={val|min,max|min,guess,max}...
Options:
--version      show program's version number and exit
-h, --help      show this help message and exit

mcrun options:
-c, --force-compile    force rebuilding of instrument
-p FILE, --param=FILE   read parameters from file FILE
-N NP, --numpoints=NP   set number of scan points
-L, --list              use a fixed list of points for linear scanning
-M, --multi             run a multi-dimensional scan
--mpi=N_CPU             spread simulation over NB_CPU machines using MPI
--machines=FILE          read machine names from FILE (MPI/grid)
--slave=HOST             execute simulation on distant HOST (SSH grid)
--optimise=COMP           Add COMP to the list of monitors to maximise
                           (optimisation criteria, requires Math::Amoeba)
--optimise-all            Maximise all monitors
--optimise-prec=PREC      relative requested accuracy of criteria (default:
                           1e-3)
--optimise-file=FILE      store optimisation results in FILE (defaults to:
                           "mcstas.dat")
--test                  execute McStas self-test and generate report
--no-cflags              disable optimising compiler flags for faster
                           compilation
--verbose                enable verbose output

Instrument options:
-s SEED, --seed=SEED      set random seed (must be: SEED != 0)
-n COUNT, --ncount=COUNT   set number of neutrons to simulate
-t, --trace                enable trace of neutron through instrument
-g, --gravitation          enable gravitation for all trajectories
-d DIR, --dir=DIR           put all data files in directory DIR
--format=FORMAT             output data files using format FORMAT (format list
                           obtained from <instr>.out -h)
--no-output-files          Do not write any data files
-i, --info                 Detailed instrument information

pkwi@pkwi-mbp15:~/tmp$
```

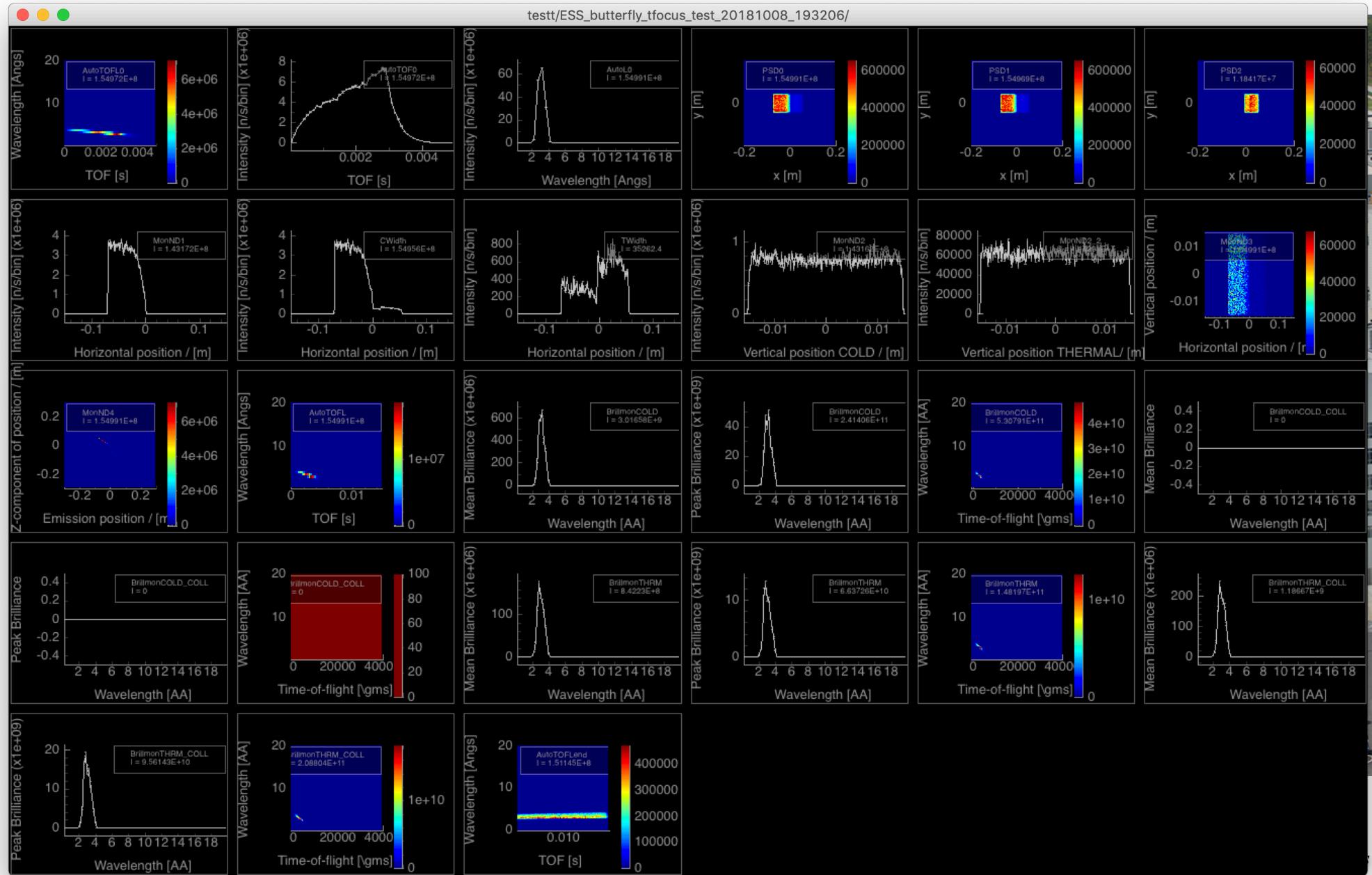
```
tmp - pkwi@pkwi-mbp15: ~/tmp - bash - 103x49
pkwi@pkwi-mbp15:~/tmp$ mcrun --help
mcrun: reading local mcstas configuration from /Users/pkwi/.mcstas/mccode_config.perl
/usr/local/bin/mcrun: reading local mcstas configuration from /Users/pkwi/.mcstas/mccode_config.perl
*** No directory given - placing data in _20160216_095914 ***
Usage: mcrun [-cpnN] Instr [-sndftgahil] params={val|min,max|min,guess,max}
mcrun options:
-c      --force-compile  Force rebuilding of instrument.
-p FILE  --param=FILE   Read parameters from file FILE.
-n COUNT --ncount=COUNT Set number of neutrons to simulate.
-N NP    --numpoints=NP  Set number of scan points.
--grid=N_CPU             Spawn simulations to multiple machine/cores grid.
                           see the documentation for more info.
--multi=N_CPU             Spread simulation over NB_CPU machines using MPI
--machines=MACHINES       Read machine names from file MACHINES (MPI/grid)
--slave=HOST              Execute simulation on distant HOST (SSH grid)
--optim=COMP               Add COMP to the list of monitors to maximize
                           (optimization criteria, requires Math::Amoeba)
--optim                         Maximise all monitors
--optim-prec=PREC           Relative requested accuracy of criteria (1e-3)
--optim-file=FILENAME       Defines filename for storing optim results.
                           (Defaults to "mcoptim_XXXX.dat")
--test                          Execute McStas selftest and generate report
--no-cflags                   Does not use CFLAGS for faster compilation

Instr options:
-s SEED, --seed=SEED        Set random seed (must be != 0)
-n COUNT, --ncount=COUNT    Set number of neutrons to simulate.
-d DIR, --dir=DIR           Put all data files in directory DIR.
-f FILE, --file=FILE         Put all data in a single file.
-t, --trace                  Enable trace of neutron through instrument.
-g, --gravitation           Enable gravitation for all trajectories.
-a, --data-only              Do not put any headers in the data files.
--no-output-files           Do not write any data files.
-h, --help                    Show help message.
-i, --info                   Detailed instrument information.
--format=FORMAT              Output data files using format FORMAT.
                           (format list obtained from <instr>.out -h)

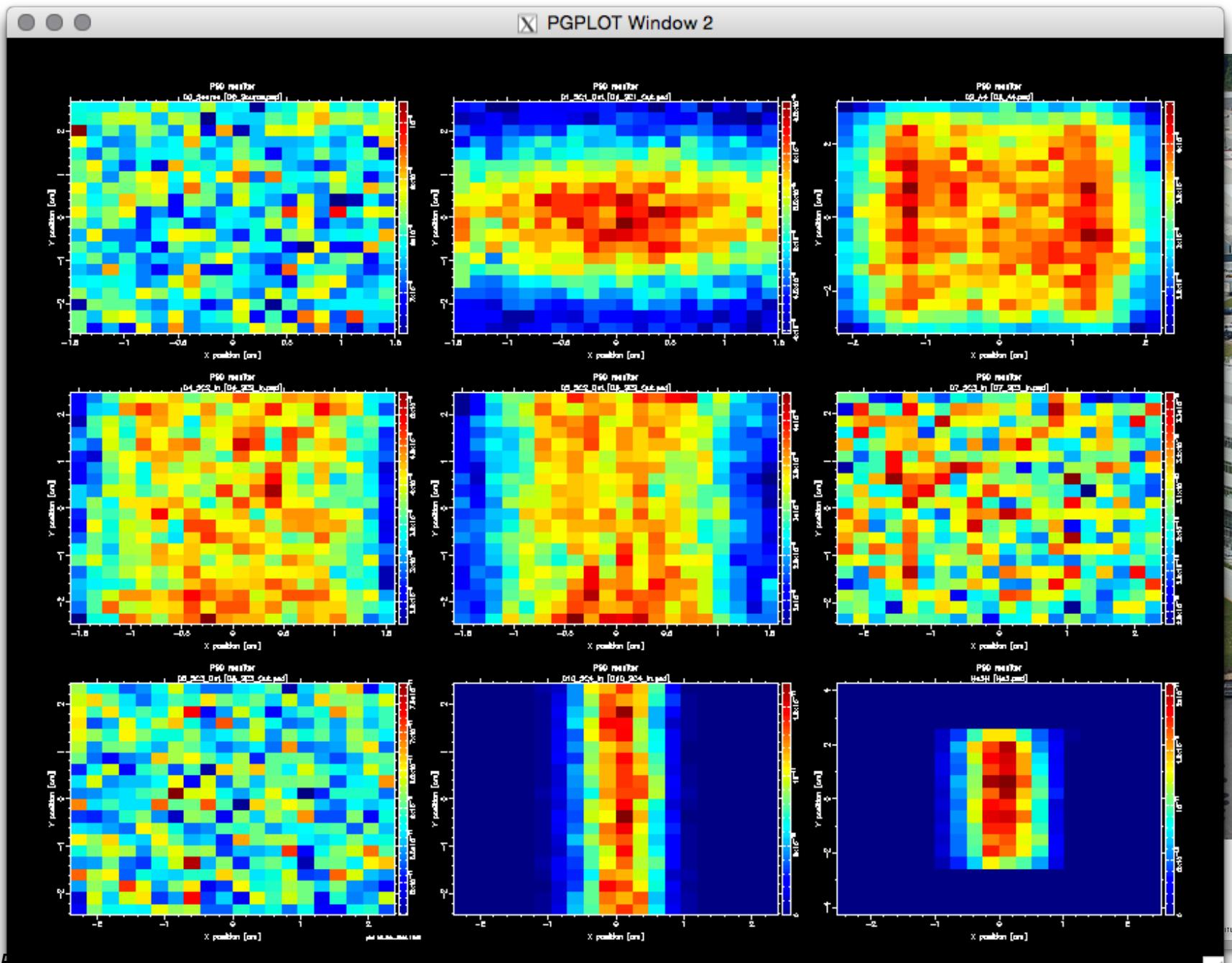
This program both runs mcstas with Instr and the C compiler to build an
independent simulation program. The following environment variables may be
specified for building the instrument:
MCSTAS          Location of the McStas and component library
                  (/Applications/McStas-2.3rc2.app/Contents/Resources/mcstas/2.3rc2).
MCSTAS_CC        Name of the C compiler
                  (cc)
MCSTAS_CFLAGS    Options for compilation
                  (-lm -g -O2 -L/usr/local/lib -lNeXus -DUSE_NEXUS )
MCSTAS_FORMAT    Default FORMAT to use for data files (PGPLOT)
SEE ALSO: mcstas, mcdoc, mcplot, mcdisplay, mcgui, mcresplot, mcstas2vitess
DOC:           Please visit http://www.mcstas.org/
** No instrument definition name given

pkwi@pkwi-mbp15:~/tmp$
```

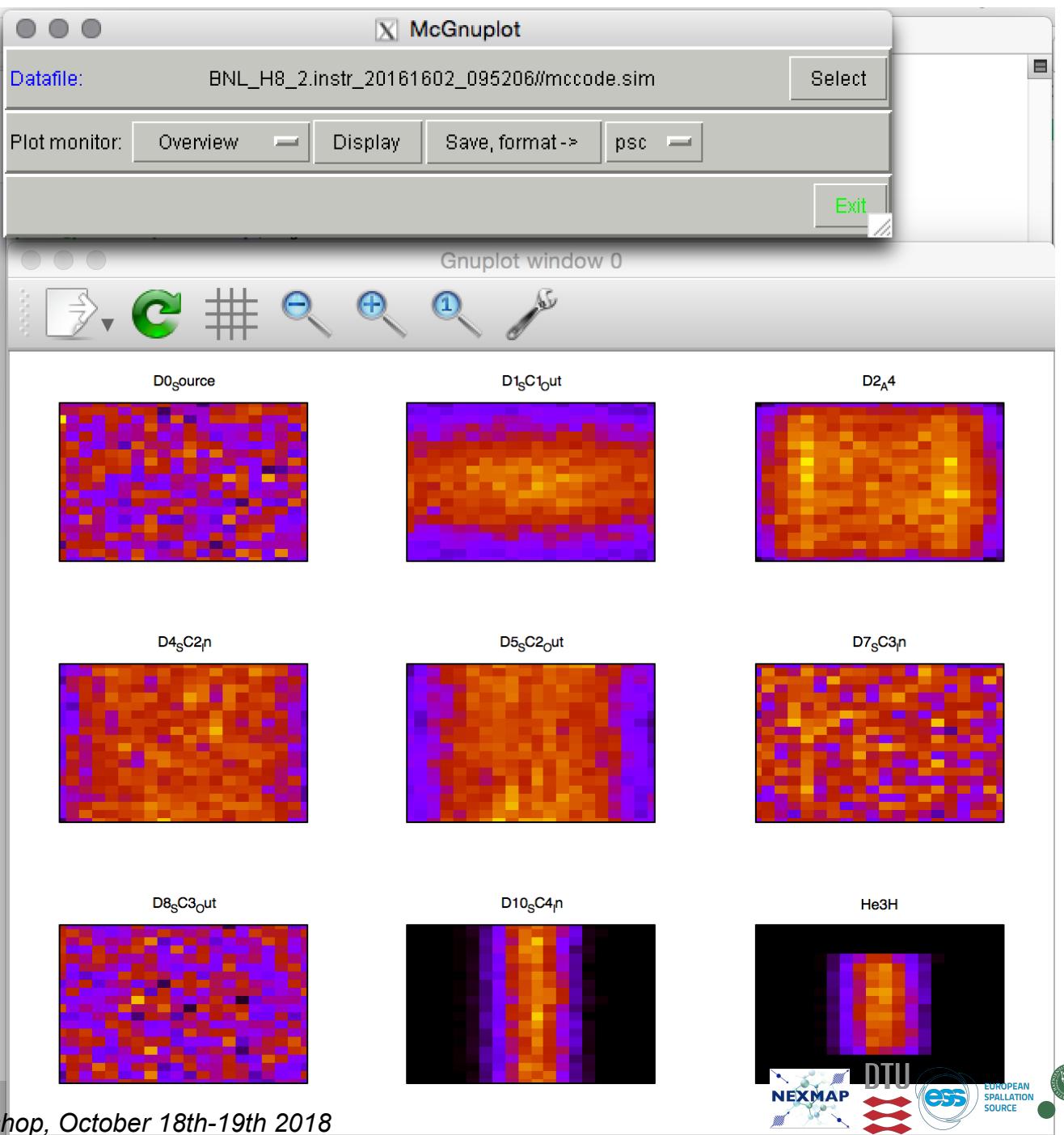
mcplot / mcplot-pyqtgraph (python)



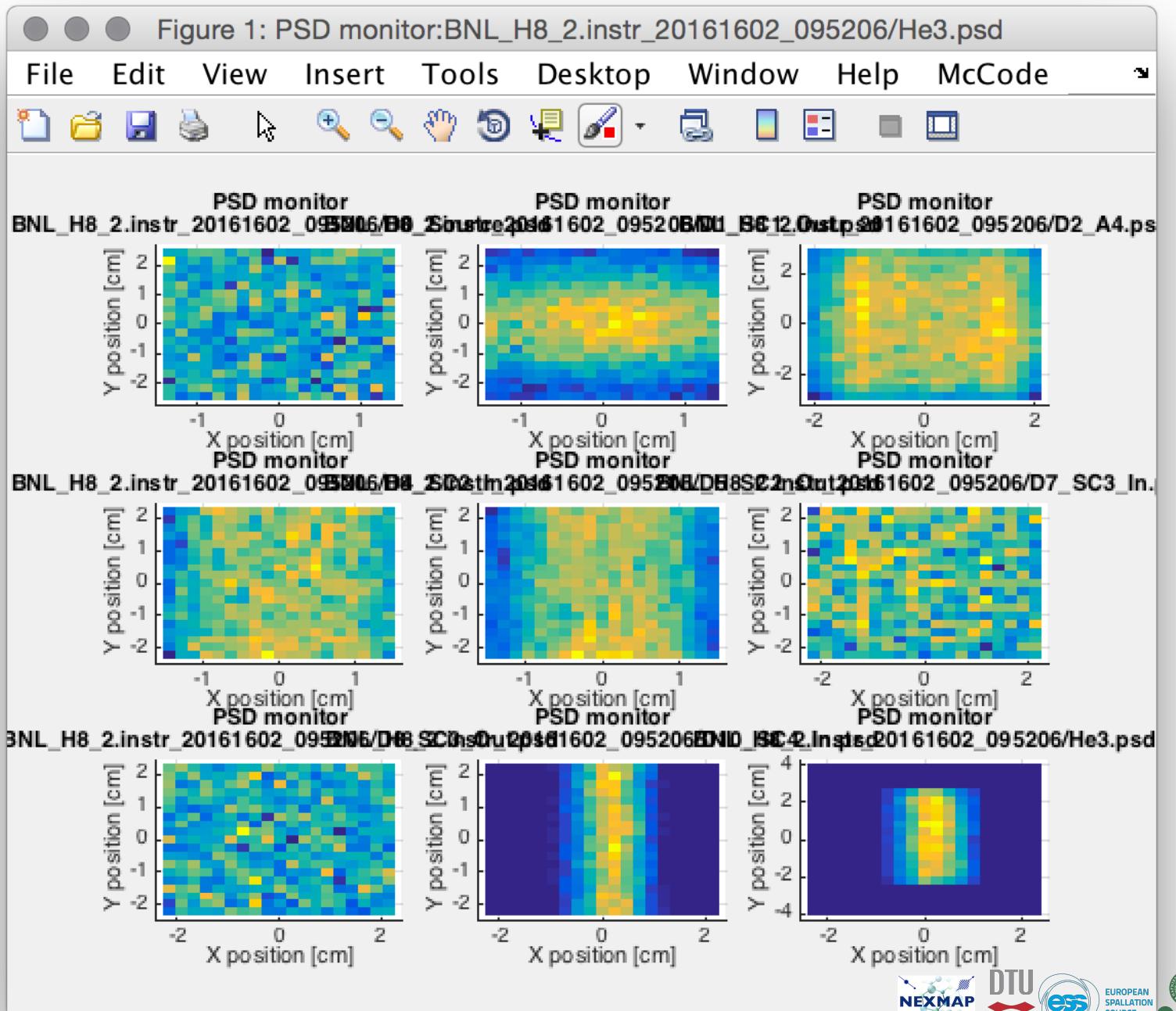
mcplot.pl/mcplot-pl (--format=PGPLOT)



mcplot.pl/mcplot-pl --format=Gnuplot



mcplot.pl/mcplot-pl –format=Matlab



mcplot-matlab (Unix only)

```
tmp — pkwi@pkwi-mbp15: ~/tmp — MATLAB — 88x50
/usr/local/bin/mcplot: reading local mcstas configuration from /Users/pkwi/.mcstas/mccode_config.perl
Click on a plot for full-window view.
Press key for hardcopy (in graphics window), 'Q' to quit
  'P' BW postscript
  'C' color postscript
  'N' PNG file
  'M' PPM file
  'G' GIF file
  'L' Toggle log10 plotting mode
  'T' Toggle contour plotting mode
  'Q' quit
```

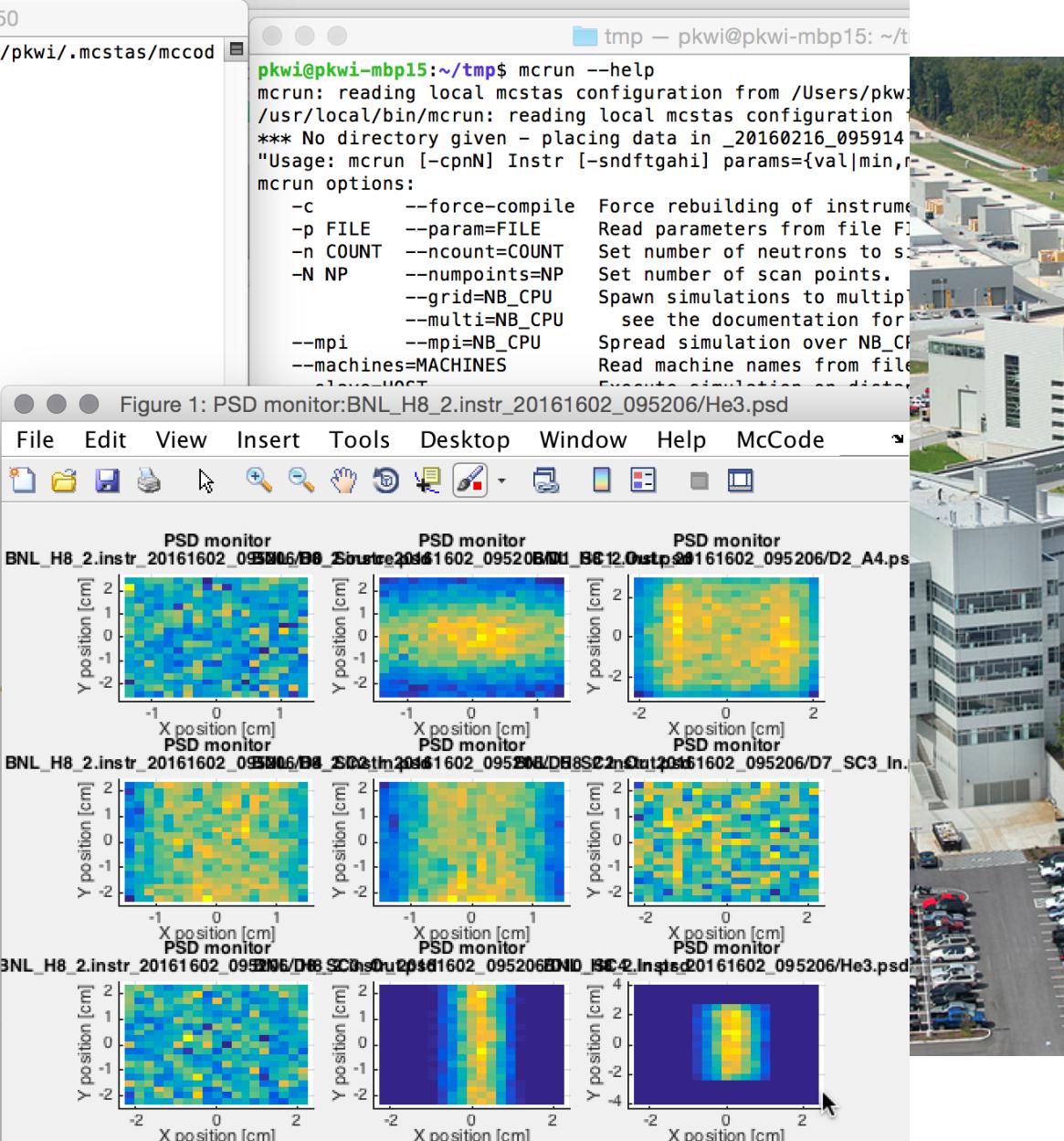
```
pkwi@pkwi-mbp15:~/tmp$ mcplot-mat BNL_H8_2.instr_20161602_095206/  
mcplot-matlab      mcplot-matplotlib-py  
pkwi@pkwi-mbp15:~/tmp$ mcplot-mat BNL_H8_2.instr_20161602_095206/  
mcplot-matlab      mcplot-matplotlib-py  
pkwi@pkwi-mbp15:~/tmp$ mcplot-matlab BNL_H8_2.instr_20161602_095206/
```

< M A T L A B (R) >

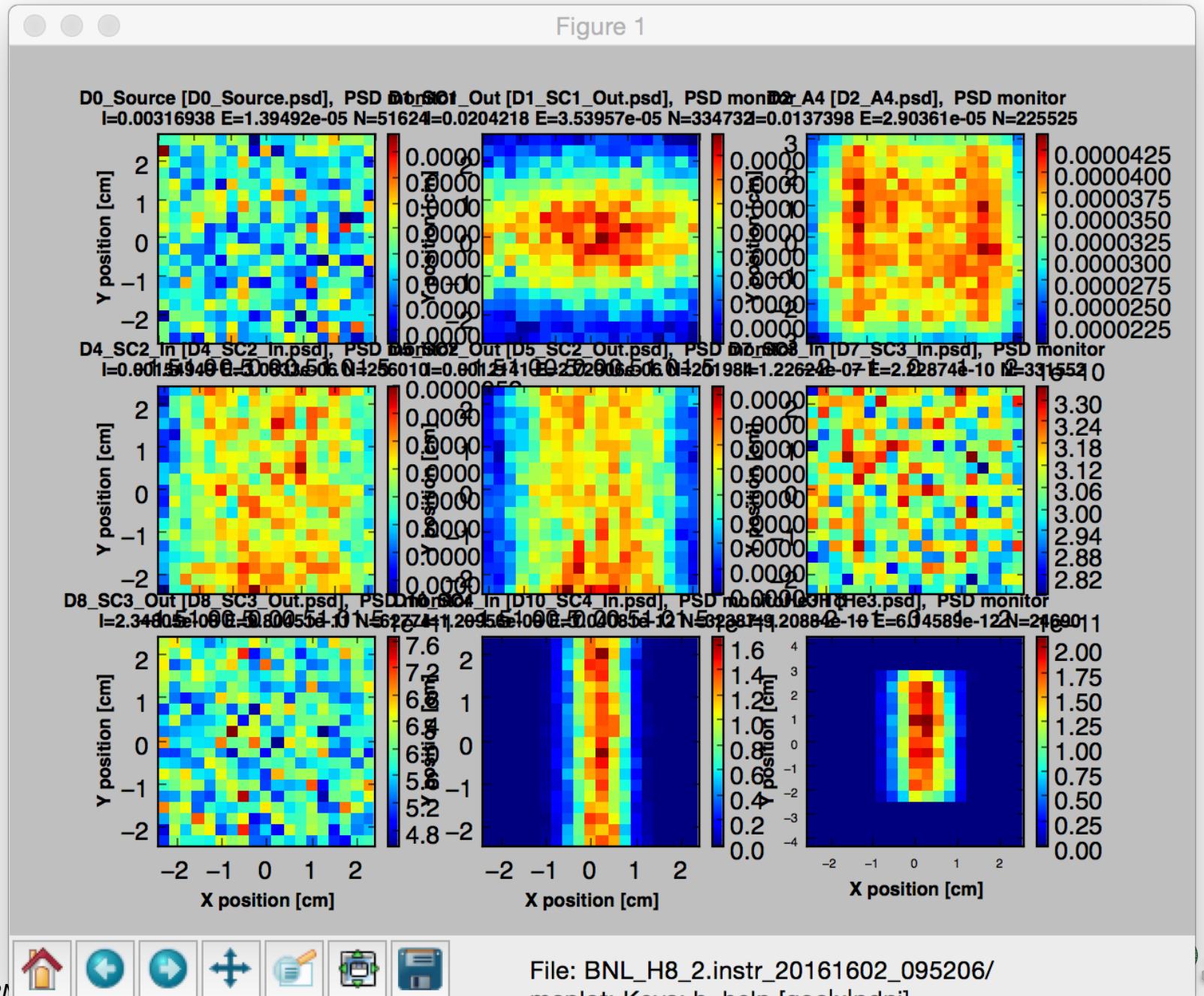
To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.

```
 Loading BNL_H8_2.instr_20161602_095206/mccode.sim (McCode simulation)
 Loading BNL_H8_2.instr_20161602_095206/D0_Source.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D1_SC1_Out.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D2_A4.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D4_SC2_In.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D5_SC2_Out.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D7_SC3_In.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D8_SC3_Out.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/D10_SC4_In.psd (McCode format)
 Loading BNL_H8_2.instr_20161602_095206/He3.psd (McCode format)
```

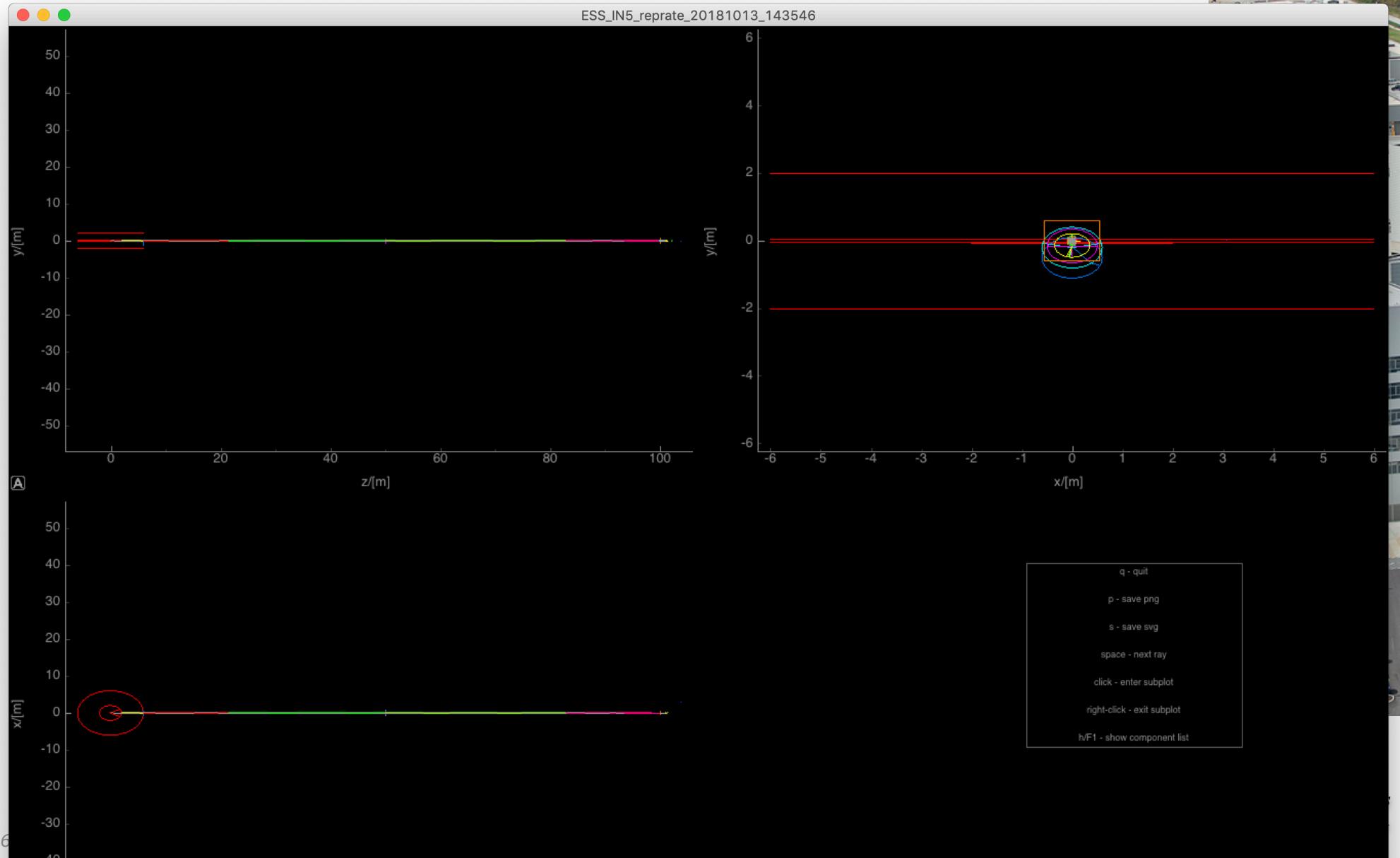
```
ans =  
Columns 1 through 5  
[1x1 struct] [1x1 struct] [1x1 struct] [1x1 struct]  
Columns 6 through 9  
[1x1 struct] [1x1 struct] [1x1 struct] [1x1 struct]  
>> □
```



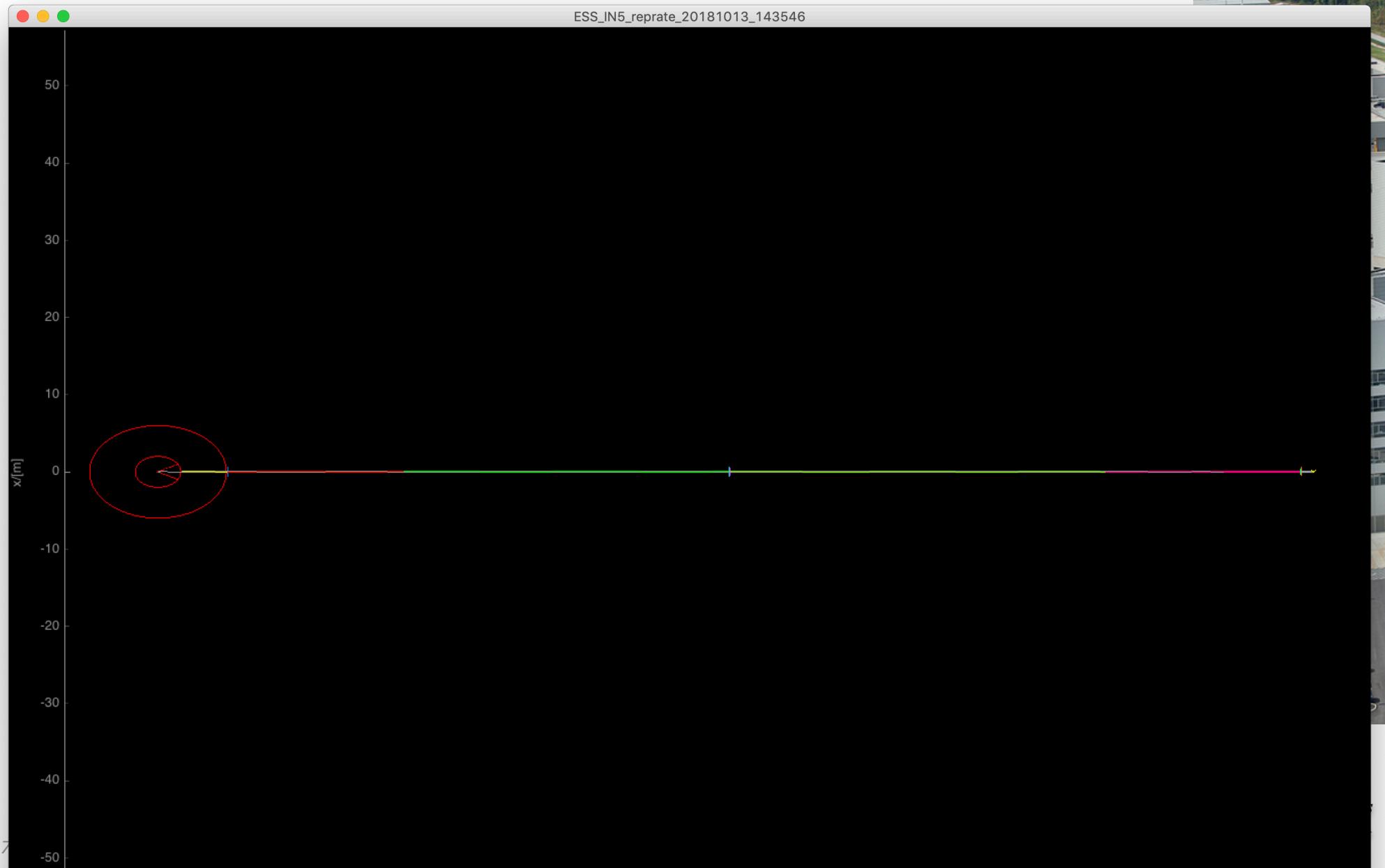
mcplot-matplotlib (python)



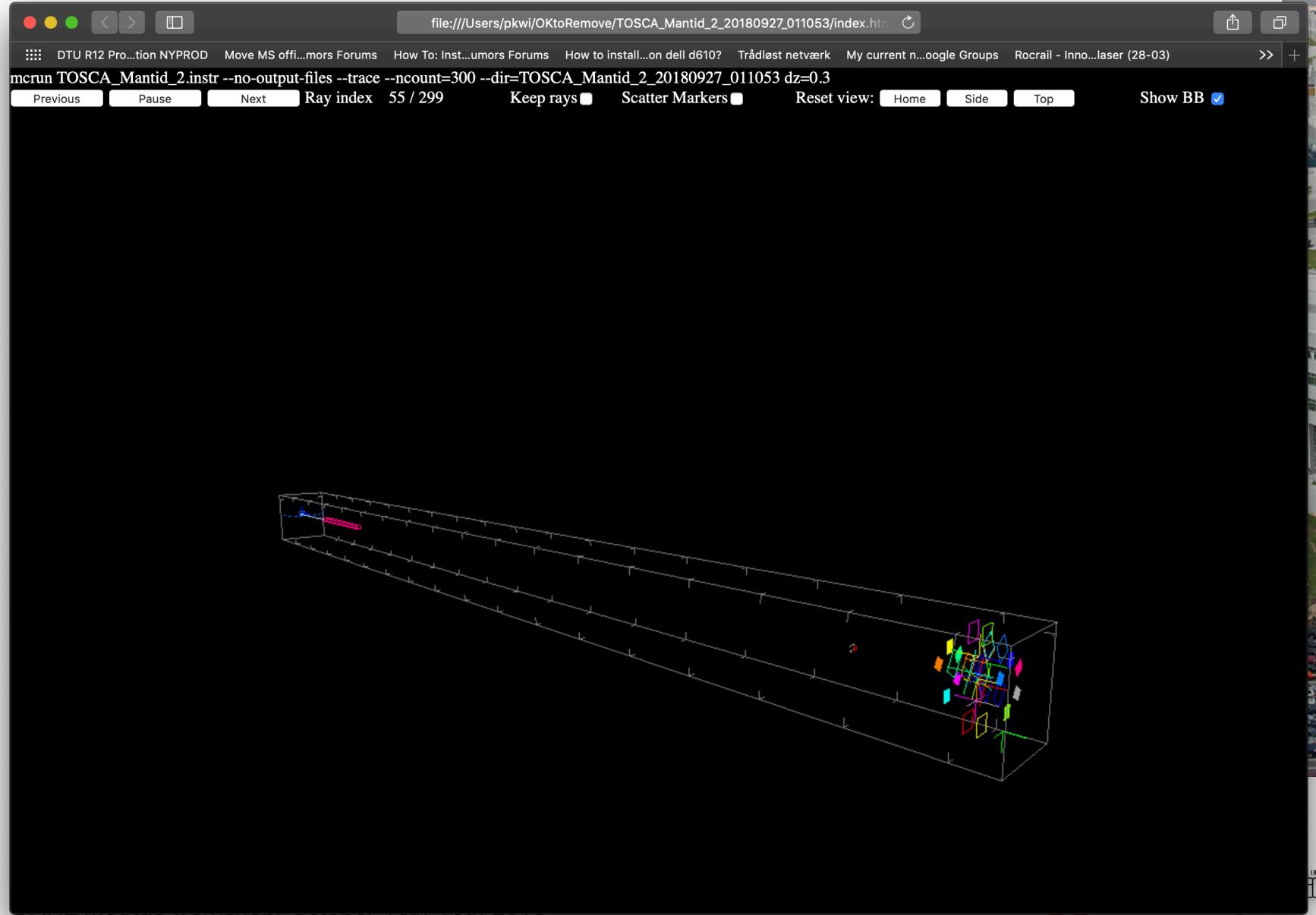
mcdisplay / mcdisplay-pyqtgraph (python)



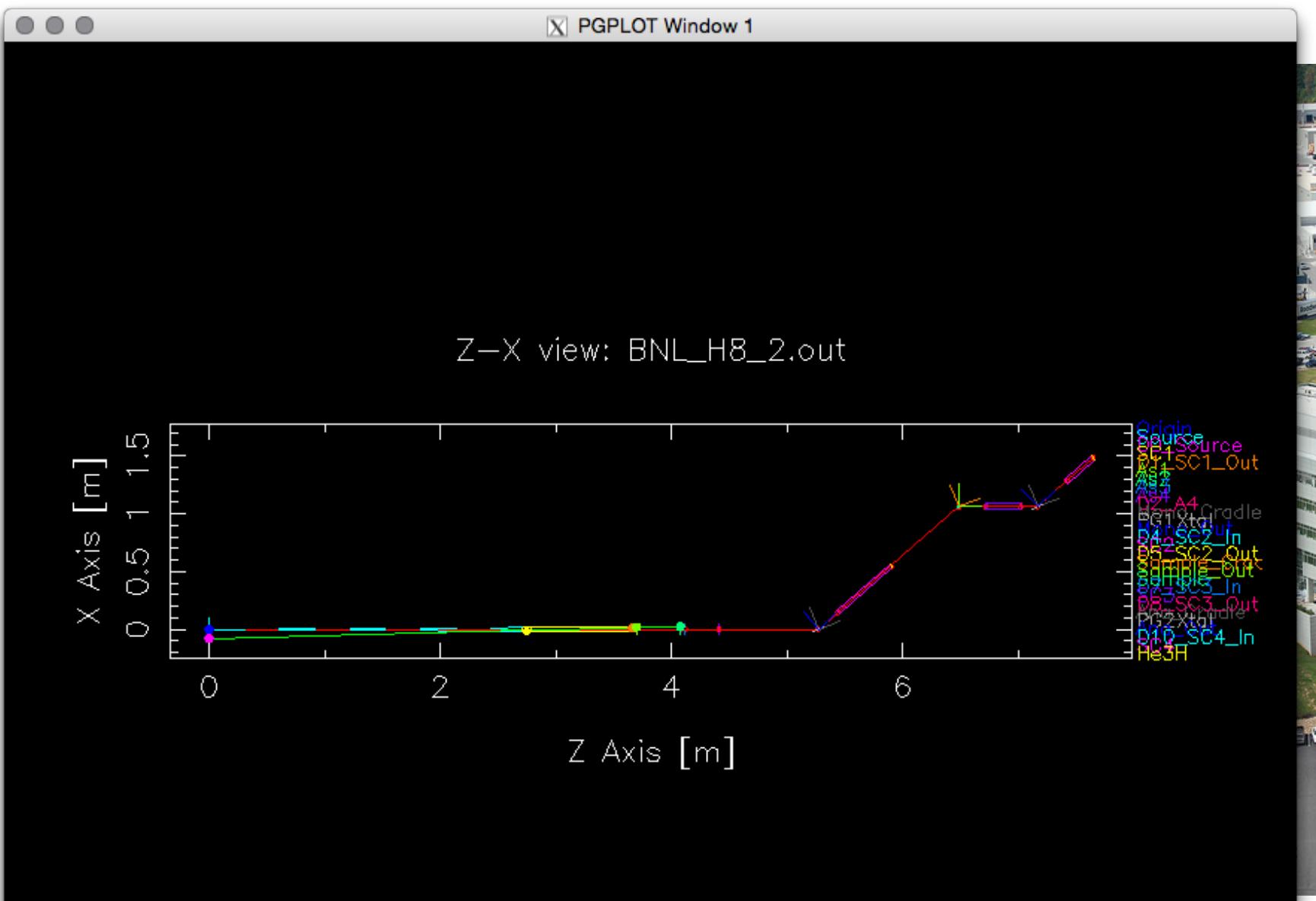
mcdisplay / mcdisplay-pyqtgraph (python)



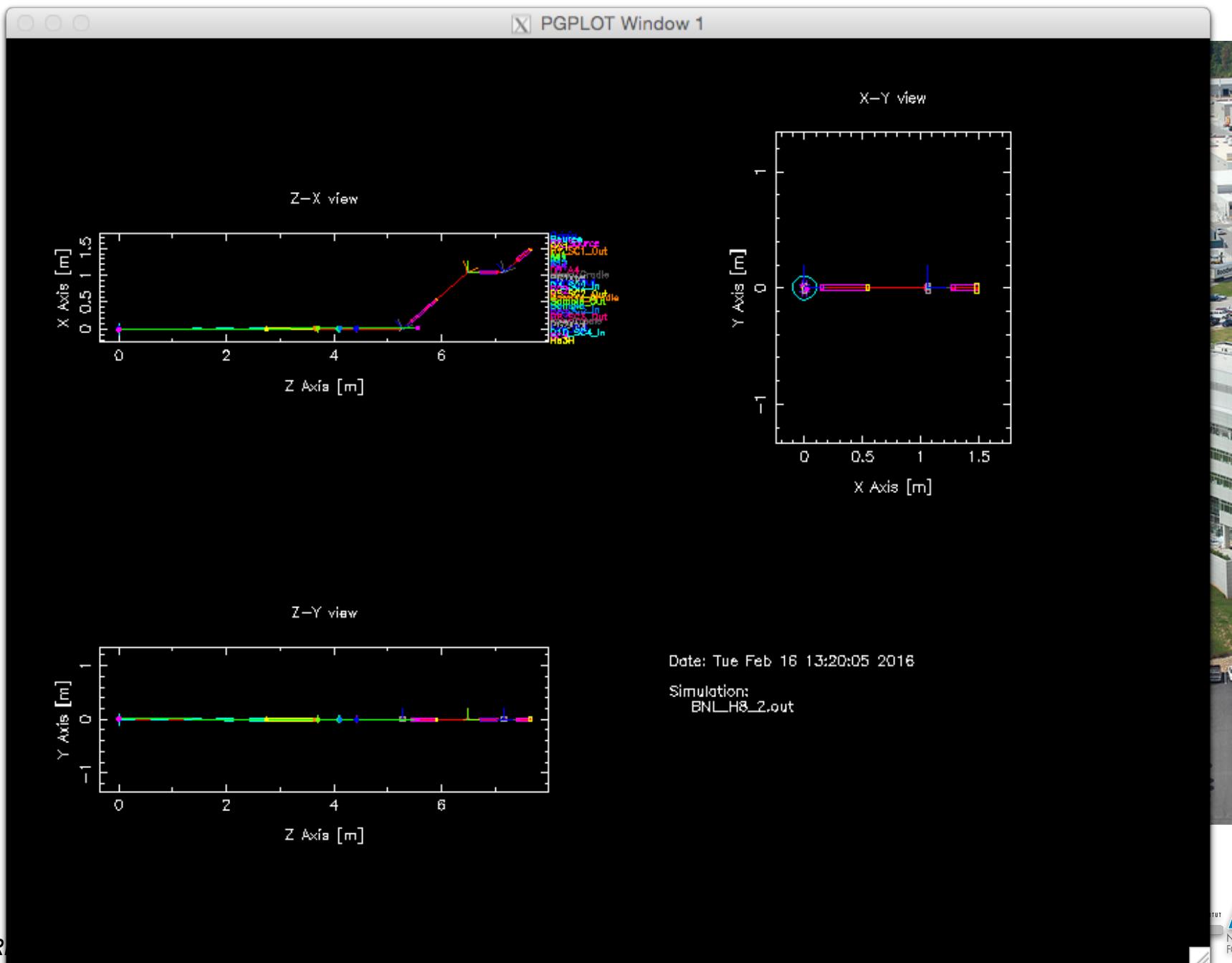
mcdisplay-webgl (python)



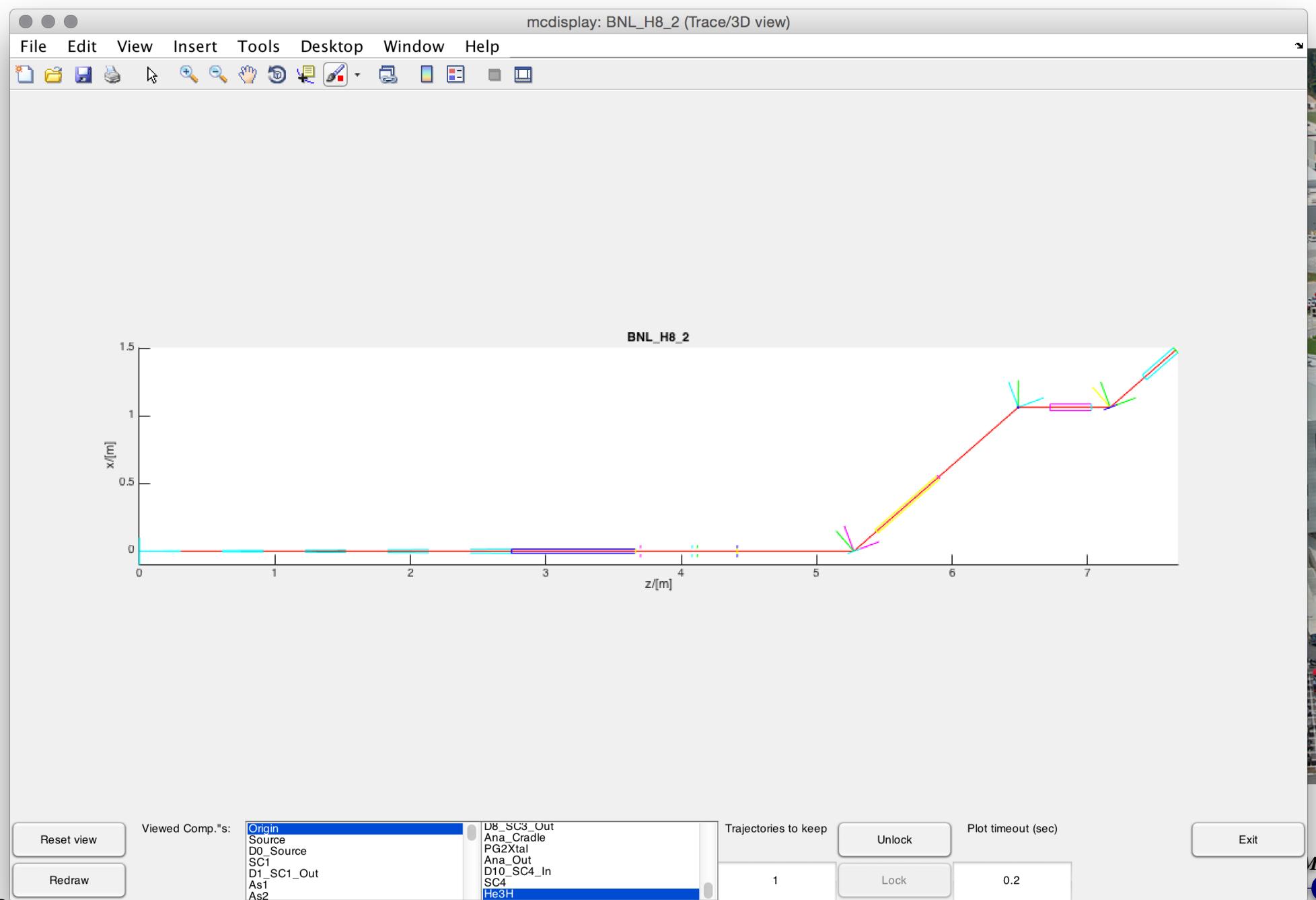
mcdisplay.pl / mcdisplay-pl



mcdisplay.pl / mcdisplay-pl with -mm

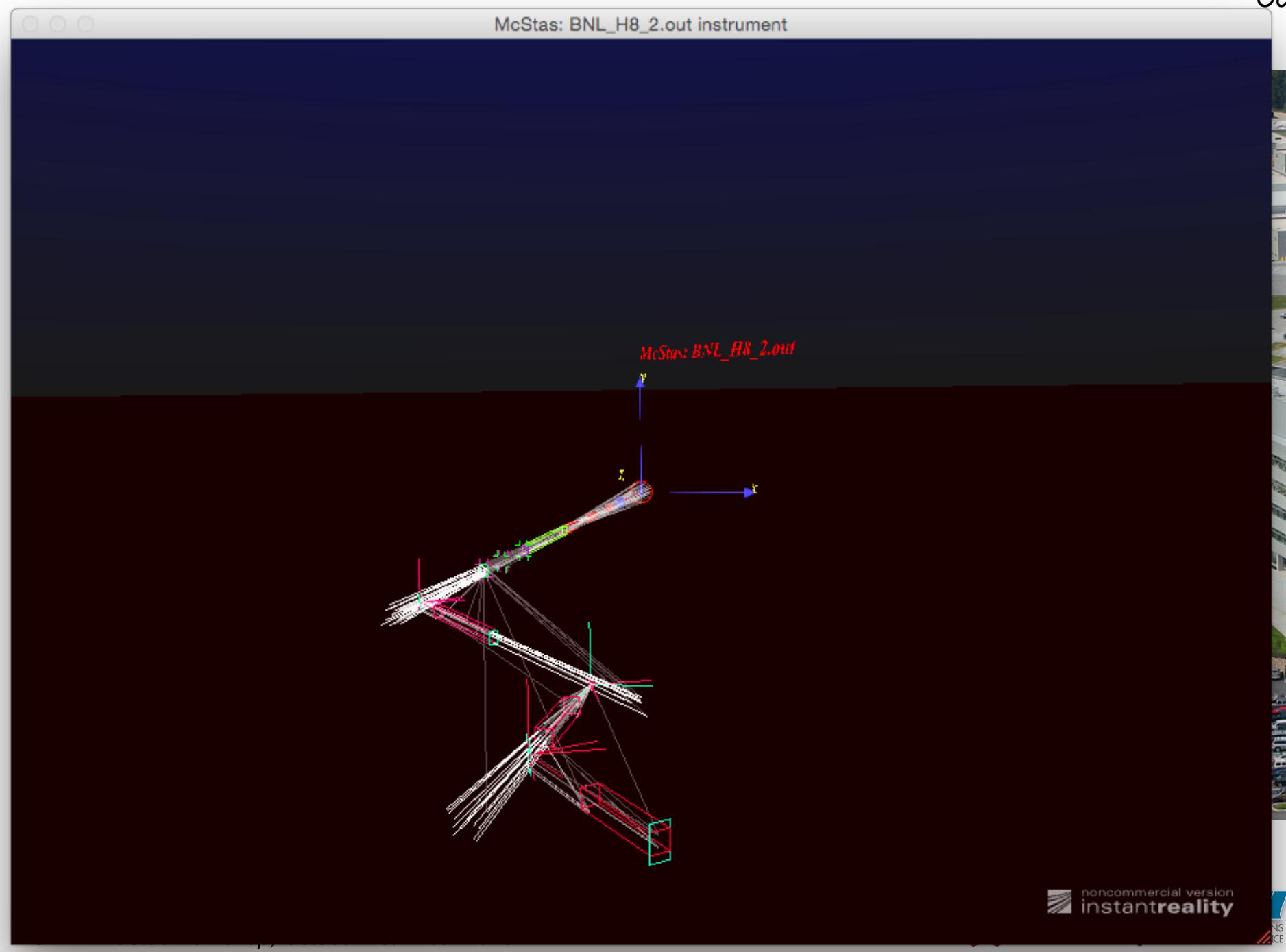


mcdisplay.pl / mcdisplay-pl --format=Matlab



October 2018

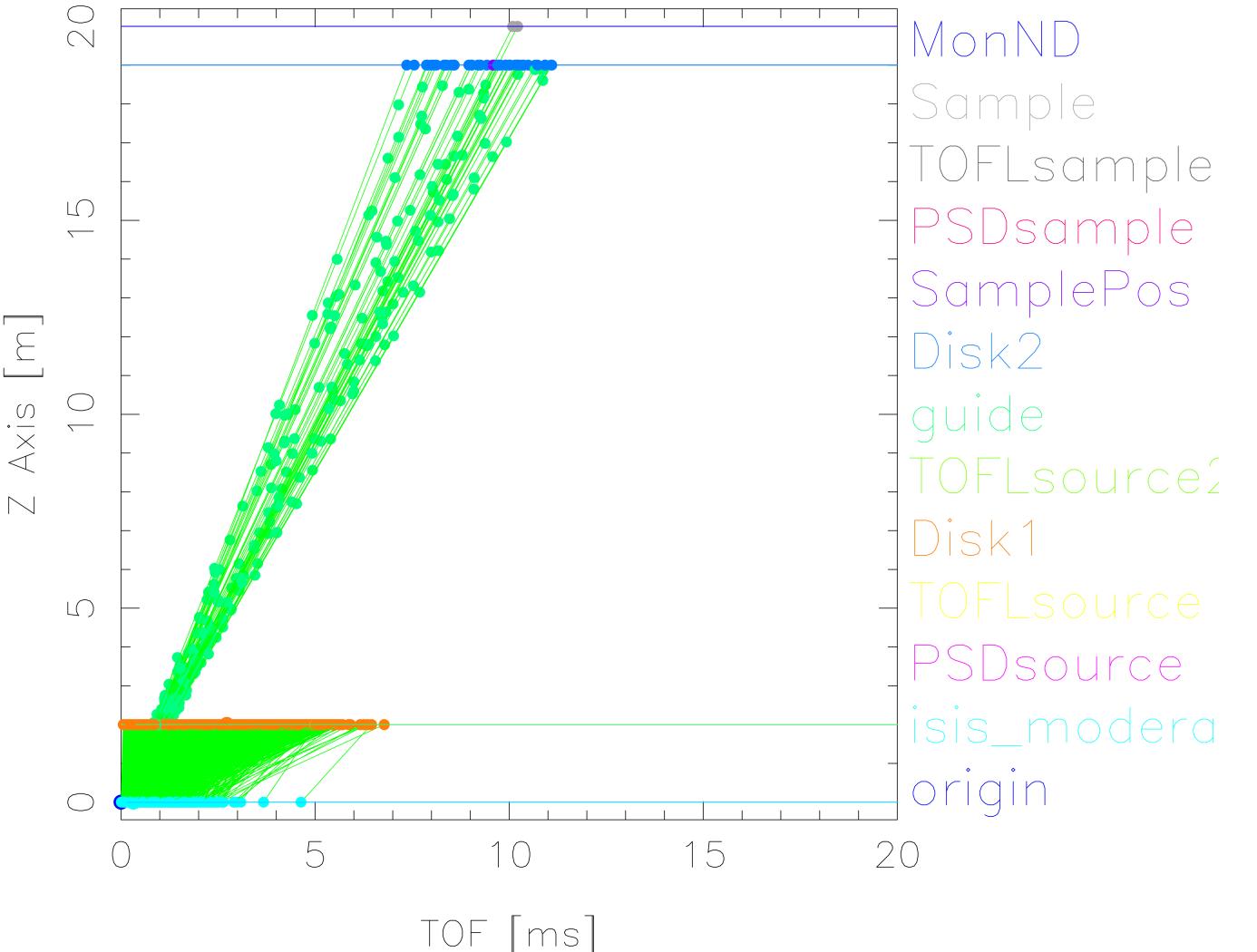
mcdisplay.pl / mcdisplay-pl --format=VRML



TOF diagram util based on mcdisplay

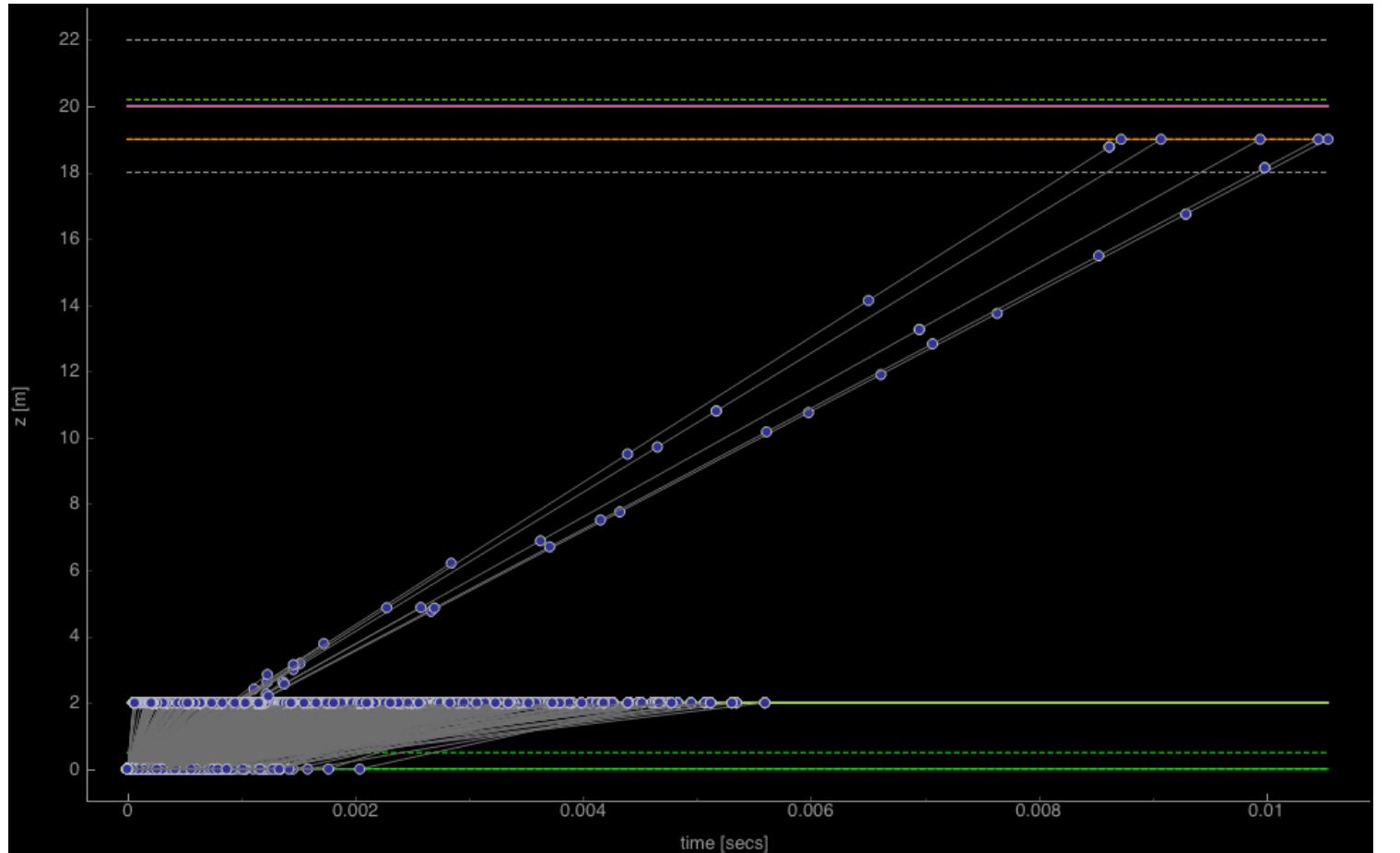
- `mcdisplay.pl --TOF --tmax=20 instrument...`

TOF diagram: STEPS.out



TOF diagram util based on mcdisplay

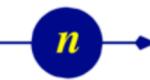
- *mcdisplay-pyqtgraph --TOF instr*



Useful links / docs

| <http://mcstas.org/links>

McStas



Overview of web resources for McStas

Get the code, report bugs etc.

- [McStas website](#)
- [McStas mailinglist subscription](#) (Please enrol!)
- [McStas Facebook page](#) (Please follow us!)
- [McStas downloads](#)
- [McStas+McXtrace GitHub](#)
- [McStas+McXtrace issues + bug reporting](#)

Neutron scattering + McStas e-learning

- [e-neutrons website](#) (free enrolment)

Tutorials, howto's, docs

- [How McStas works - in 2 minutes](#)
- [Tutorial: Build a SANS](#)
- [Tutorial: Build a diffractometer](#) (outdated in certain parts)
- [McStas user manual - Better use `mcdoc -m` in the terminal!](#)
- [McStas component manual - Better use `mcdoc -c` in the terminal!](#)
- [McStas component docs - Better use `mcdoc` in the terminal!](#)
- [McStas sample model functionality matrix](#) (not fully up to date)
- [McStas and McXtrace GitHub wiki - tutorials, guides and more](#)

| <https://github.com/McStasMcXtrace/McCode/wiki>

Documentation on the McCode tools

- [User documentation for the 2017- Python tool set](#)
- [mcrun variants - table overview](#)
- [mcplot variants - table overview](#)
- [mcdisplay variants - table overview](#)



October 2018

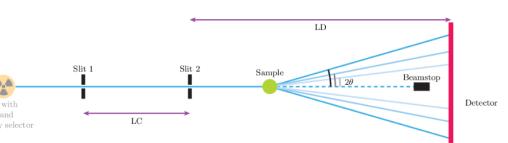
Web interface @ e-neutrons.org

sim.e-neutrons.org

Instrument

Logged in as pwillendrup (see recent simruns) [Logout](#)

SANSsimple (click for documentation)



Source with guides and velocity selector

Slit 1

Slit 2

Sample

Beamstop

Detector

LD

LC

2θ

Parameters for SANSsimple

pinhole_rad [m]	0.004	radius of the collimating pinholes (0.004)
LC [m]	3	length of the collimator – distance between pinholes (3)
LD [m]	3	distance between the last pinhole slit and detector (3)
Lambda [Angs]	6	Average wavelength traced from source (6)
DLambda [Angs]	0.6	Wavelength band +/- traced from source (0.6)
R [AA]	400	radius of the hard, monodisperse spheres in the sample (400)
dR [AA]	0	Normal variance of Radius (0)
PHI [1]	0.01	Volumefraction of the hard, monodisperse spheres in the sample (0.01)
Delta_Rho [fm/AA^3]	0.6	Volume specific scattering length density contrast of the hard, monodisperse spheres in the sample as compared to the solution (0.6)
Qmax [AA^-1]	0.3	Maximum scattering vector allowed by geometry to hit the detector area (0.3)
BEAMSTOP [0/1]	1	If set, the beamstop is inserted in front of the detector in order to block the transmitted beam (1)
SAMPLE [0/1]	1	If set, a sample of spheres or spherical shells is inserted (1)

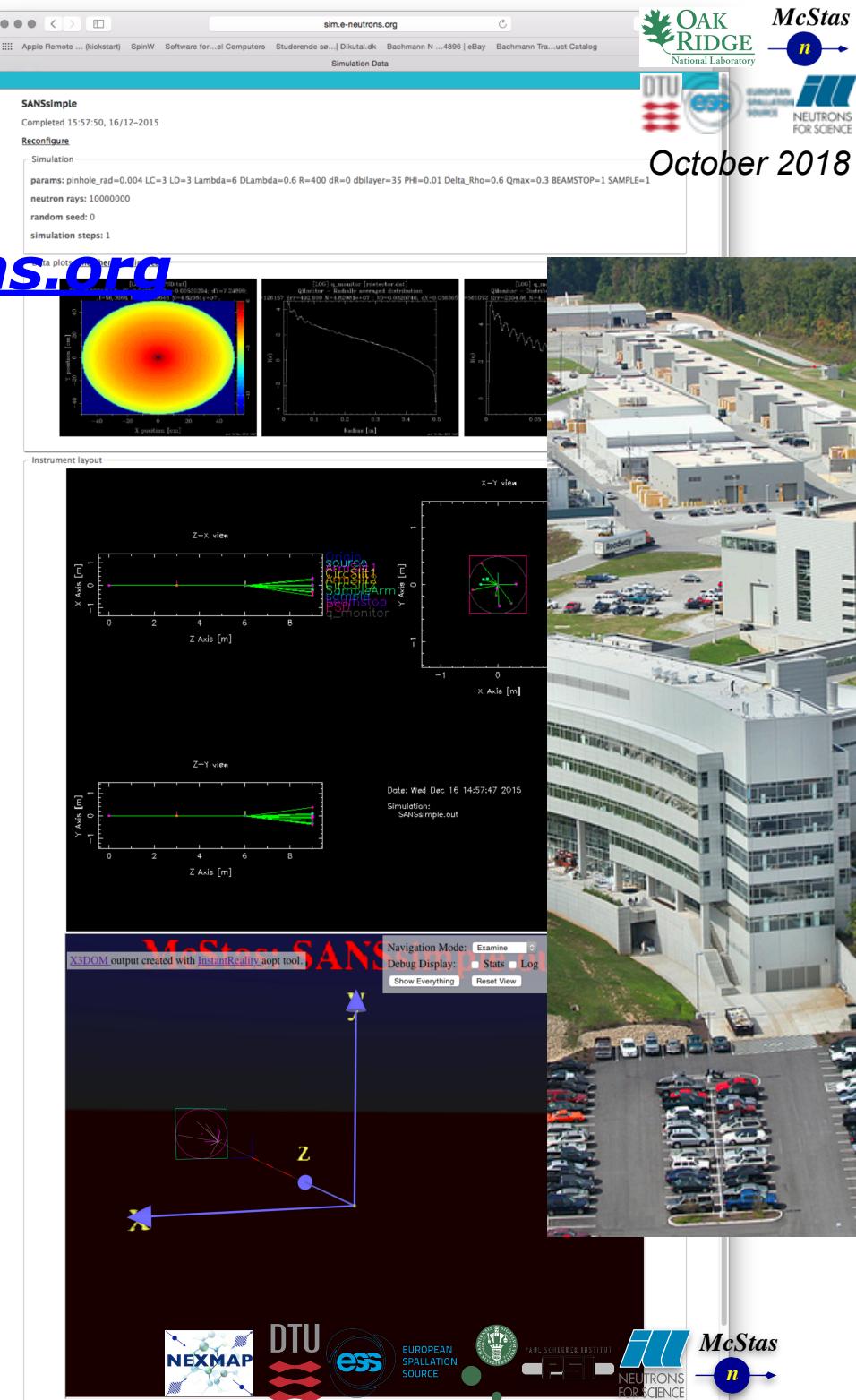
Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0

Start simulation run [Run](#)

A web-based interface for **McStas**.

All contents is provided under the terms of [!\[\]\(8a482f7d703b2f3a21bcbafdaced4511_img.jpg\)](#)



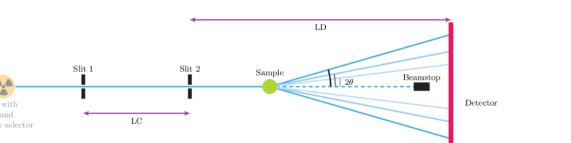
October 2018

Web interface @ [e-neutrons.org](http://sim.e-neutrons.org)

Logged in as pwillendrup (see recent simruns) [Logout](#)

Instrument

SANSsimple (click for documentation)



Parameters for SANSsimple

pinhole_rad [m]	0.004	radius of the collimating pinholes (0.004)
LC [m]	3	length of the collimator (3)
LD [m]	3	distance between the sample and the detector (3)
Lambda [Angs]	6	Average wavelength (6 Angstroms)
DLambda [Angs]	0.6	Wavelength spread (0.6 Angstroms)
R [AA]	400	radius of the hard, monodisperse spheres in the sample (400)
dR [AA]	0	Normal variance of Radius (0)
PHI [1]	0.01	Volumefraction of the hard, monodisperse spheres in the sample (0.01)
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simulation steps:	1
random seed:	0

Start simulation run

[Run](#)

A web-based interface for McStas.

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Courses

- Introduction to Neutron Scattering**
High-guidance self study
- Introduction to Neutron Scattering**
Open course for blended learning
- Muon Spin Spectroscopy**
A course on a complementary technique to neutron scattering

INTRODUCTION TO NEUTRON SCATTERING - SELF STUDY

This course contains 10 high-guidance modules on master-level physics.

Each module takes approximately 10-20h to complete.

[READ MORE](#)

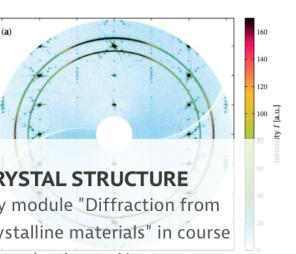
Science cases

- Finding crystal structure**
Chemistry of materials
- Characterising liposomes in suspension**
Life sciences
- Characterising magnetic order**
Magnetic and electronic phenomena

CRYSTAL STRUCTURE

Try module "Diffraction from crystalline materials" in course "Introduction to Neutron Scattering"

[READ MORE](#)



Exercise taster

[Problem: Fourier transform](#)

What happens if a scatterer applies the Fourier transform of the distribution of scattering centers (sources, electrons, spins) within the material. The scattered intensity (the scattering function) is given by the Fourier transform of the scattering function $\rho(r)$ written as:

$$F(q) = \int \rho(r) e^{iq \cdot r} dr,$$

where $\rho(r)$ is the function in real space at even positions r , and q is a coordinate in scattering space (which in scattering terms usually is called "reciprocal space"), $q^2 = q_x^2 + q_y^2 + q_z^2$.

We can consider a one-dimensional case, i.e. all particles (scattering centers) are positioned on a line, and correspondingly only calculate the one-dimensional Fourier transform. We assume further that all particles (n particles) $\rho(r) = \rho_0$.

Contents (here)

- 1 Problem
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- 4 Solution
- 5 Quiz
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We


e-neutrons

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Username: pwillendru Password: [Login](#)

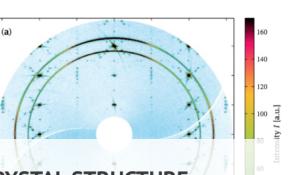
Courses

- Introduction to Neutron Scattering**
High-guidance self study
- Introduction to Neutron Scattering**
Open course for blended learning
- Muon Spin Spectroscopy**
A course on a complementary technique to neutron scattering

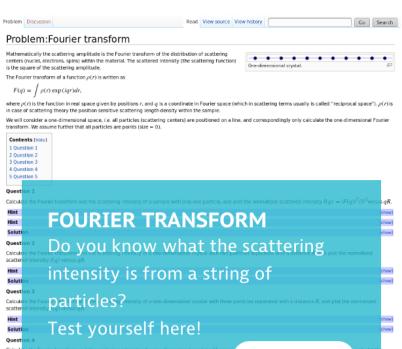
Online-course on neutron scattering available!

Science cases

- Finding crystal structure**
Chemistry of materials
- Characterising liposomes in suspension**

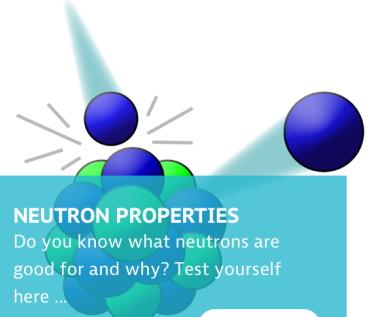


Exercise taster



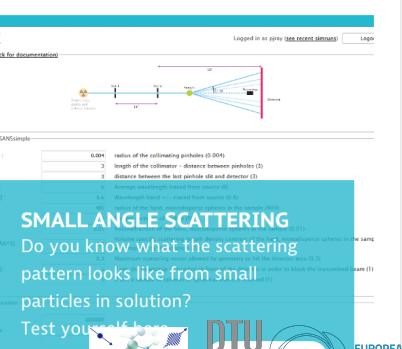
FOURIER TRANSFORM
Do you know what the scattering intensity is from a string of particles?
Test yourself here! [READ MORE](#)

Quiz taster



NEUTRON PROPERTIES
Do you know what neutrons are good for and why? Test yourself here ... [READ MORE](#)

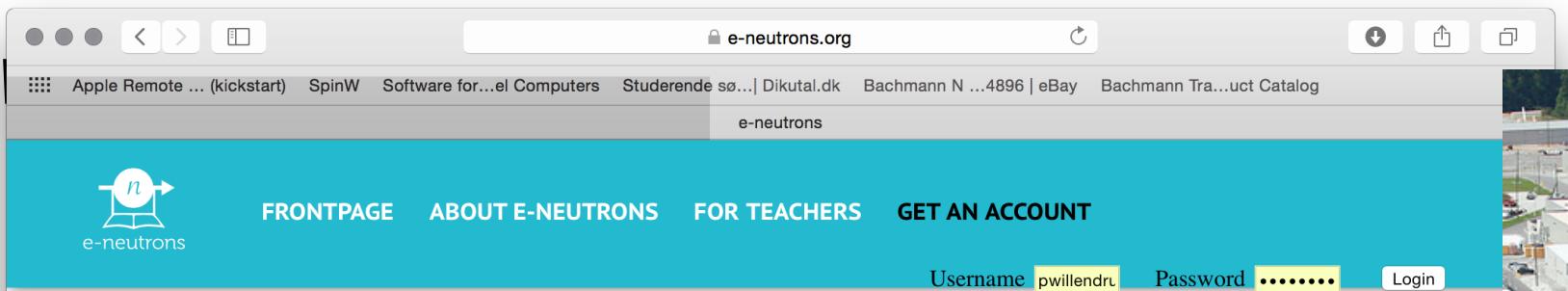
Simulation taster



SMALL ANGLE SCATTERING
Do you know what the scattering pattern looks like from small particles in solution?
Test yourself here! [READ MORE](#)



October 2018



The available selection of courses is visible at this [Moodle page](#). The list below uses the "short" naming convention for courses, i.e.

- ns-intro="Introduction to neutron scattering"
- ns-intro-selfstudy="Introduction to neutron scattering – self study"
- musr="Introduction to muon spin resonance"

Please fill in the form, indicating your personal data and requested courses.

If you have an account already and want to change your password, please visit our [Password change service](#)

Please avoid special characters like the Danish æ,ø and å in this prototype

I'm not a robot 
Privacy - Terms

First Name:	<input type="text"/>
Last Name:	<input type="text"/>
Email:	<input type="text"/>
Requested username:	<input type="text"/>
<input type="checkbox"/> intro-ns-selfstudy <input type="checkbox"/> intro-ns <input type="checkbox"/> musr	
<input type="button" value="Submit"/>	

October 2018

The screenshot shows a web browser window for e-neutrons.org. The page has a teal header with the e-neutrons logo, navigation links for FRONTPAGE, ABOUT E-NEUTRONS, FOR TEACHERS, and GET AN ACCOUNT, and a login form with fields for Username (pwillendru) and Password (redacted). To the right of the header is a large image of the European Spallation Source facility.

The available selection of courses is visible at this [Moodle page](#). The list below uses the "short" naming convention for courses, i.e.

- ns-intro="Introduction to neutron scattering"
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Please avoid special characters!

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 reCAPTCHA
Privacy - Terms

First Name:

Last Name:

Email:

Requested username:

intro-ns-selfstudy

intro-ns

musr

6 McStas various utils

- *Hidden gems and useful little things...*
- + *Disclaimers and tips for the next couple of days...*



cif2hkl



- Util for generating McStas style “laz/lau” reflection lists from CIF file
- Based on CrysFML from the ILL (FullProf)
- Compile for your system from
<https://github.com/McStasMcXtrace/McCode/tree/master/tools/other/cif2hkl>
- (May also get included in McStas 2.4)

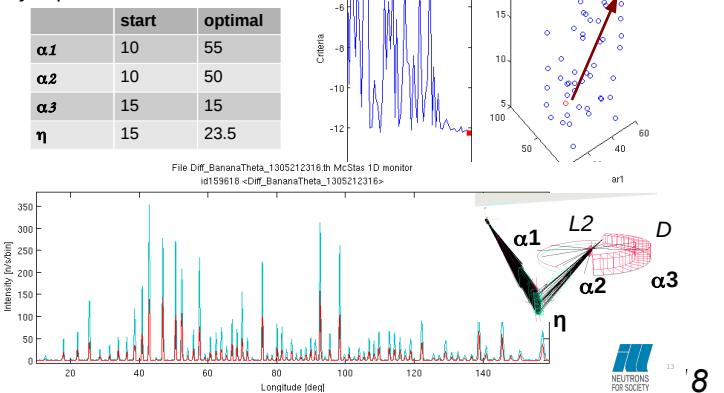
iFit optimiser (<http://ifit.mccode.org>)

- General data / optimisation framework
- ~ Modern “spec_nd”
- Matlab based, but does not require matlab (binary distribution also)
- Reads and plots McStas
- Can run McStas as a “cost function”, varying instrument parameters



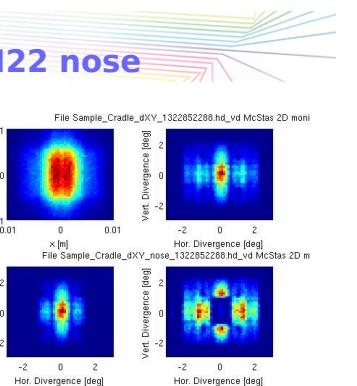
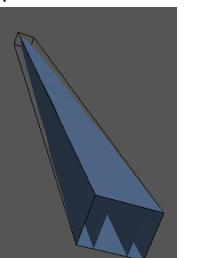
iFit/McStas: example: diffractometer

Space: 4 parameters
 Execution: 45 minutes on 2 cores
 Many equivalent solutions.



iFit/McStas: example: IN22 nose

- Gain a factor 3 in flux for 50 kE.
- No need to use high m coating for top/bottom $\rightarrow m=4$
 - $m=6$ to $m=5$ only reduces flux by 1%.
 - Nose 87 cm long. Profile is not fully parabolic.



Cluster utility scripts



- *mcsub cluster scripts*

```
./mcsub_slurm.pl
Usage: ./mcsub_slurm.pl [options] [mcrun params]
-h      --help          Show this help
-rN     --runtime=N     Specify maximum runtime (hours) [default 1]
-qQNAME --queue=QNAME  Specify wanted SLURM queue [default 'express']
-e<mail> --email=<mail> Specify address to notify in reg. sim status [default none]
--nodes=NUM           Specify wanted number of nodes [default 1]
--name=NAME           Specify slurm job name [default
"McSub_<USERNAME>_<TIMESTAMP>"]
```

After running `./mcsub_slurm.pl NAME.batch` is ready for submission using the `sbatch` command

- *Takes a “mcrun commandline”*

- *Writes batch file “template” for use with PBS or slurm cluster queue systems*

- <https://github.com/McStasMcXtrace/McCode/tree/master/tools/cluster-scripts>

Vitess - compatibility

- Utility script for converting Vitess reflectivity files for use with McStas (https://github.com/McStasMcXtrace/McCode/blob/master/tools/other/Refl_Vitess2McStas.sh)
- mcstas2vitess generates Vitess module + tcl snippet from McStas component (poor docs, will improve)



Next: Time for exercises

Forming groups

Suggestion for Thursday-Friday exercises:

- Often sitting with a colleague is helpful
- Form teams of two people for the exercises
- Try to gather complementary knowledge by teaming up with someone from a different work area



Next: Exercises

Disclaimers

- We will likely find new and interesting bugs as we move along... :-)*



Programme is flexible - don't get frustrated if we lag behind, we will either adapt or catch up later!



- Much of the teaching material is new / adapted, so there may be inconsistencies / confusion in some parts... :-)*

