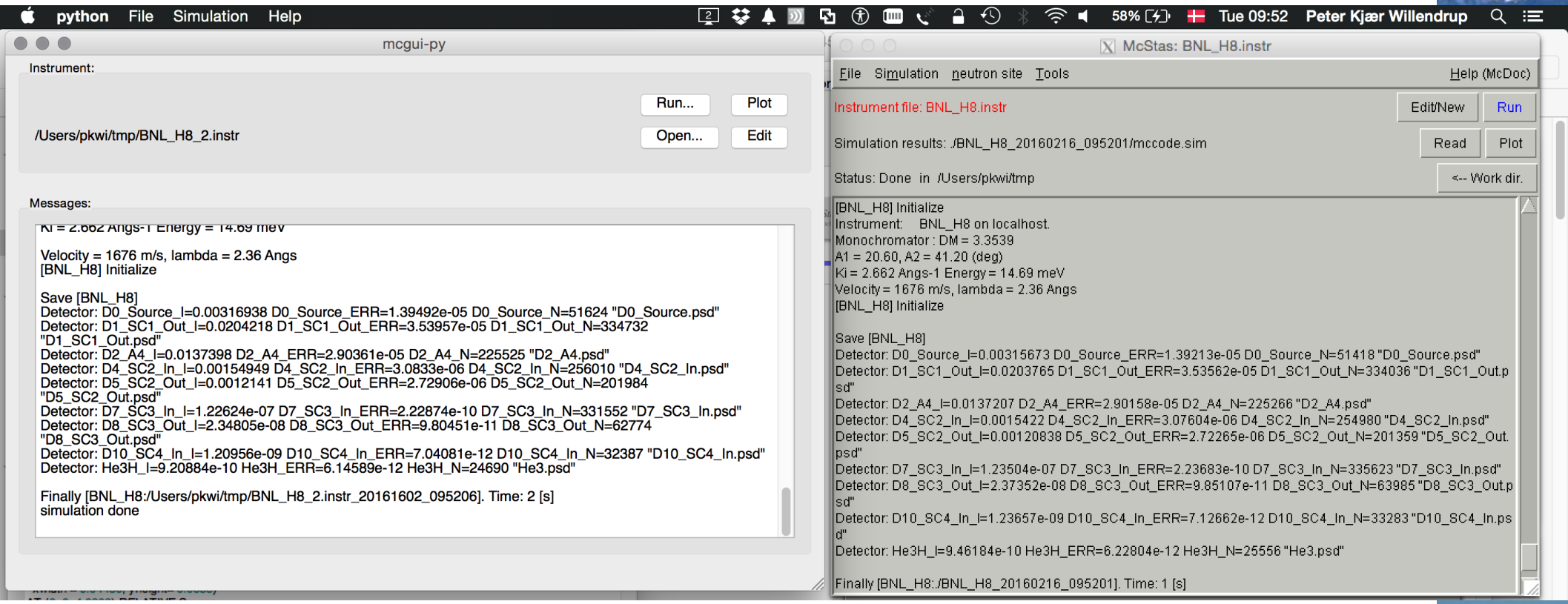
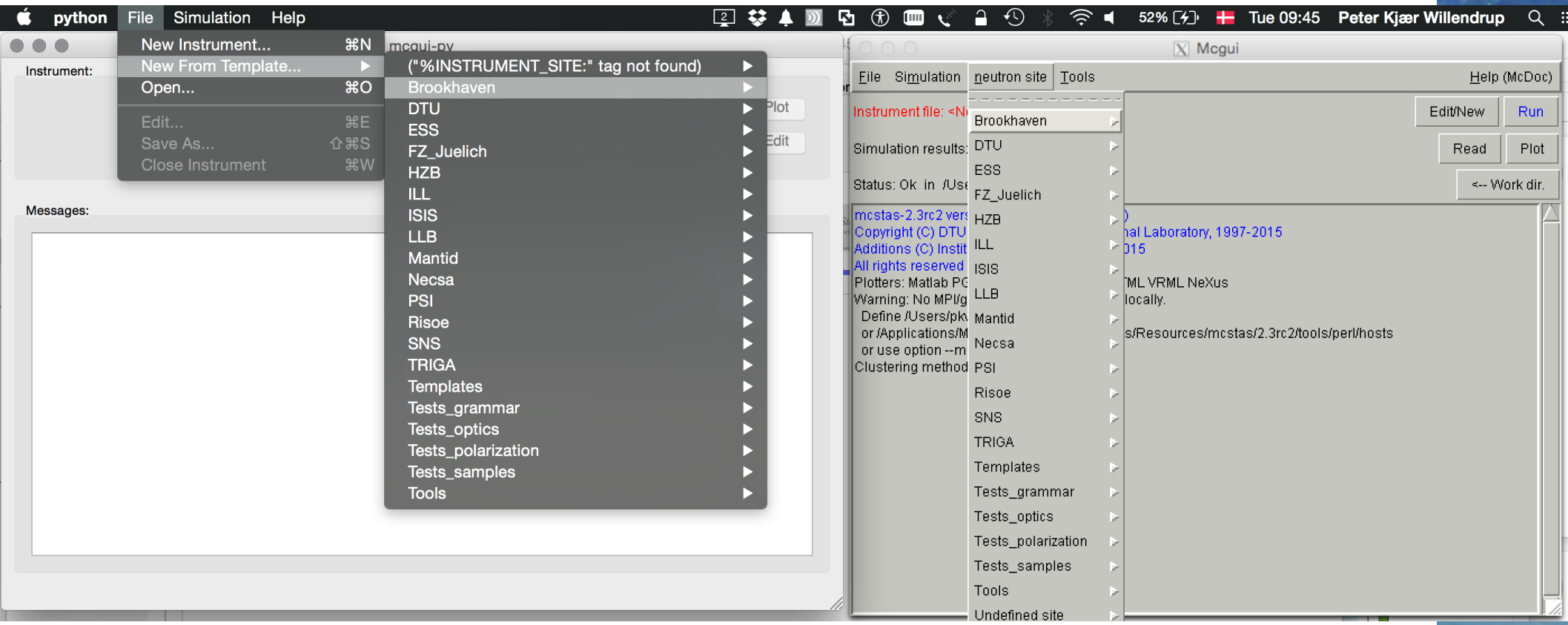
Extras - quick tour of available tools

mcgui - pl vs py versions



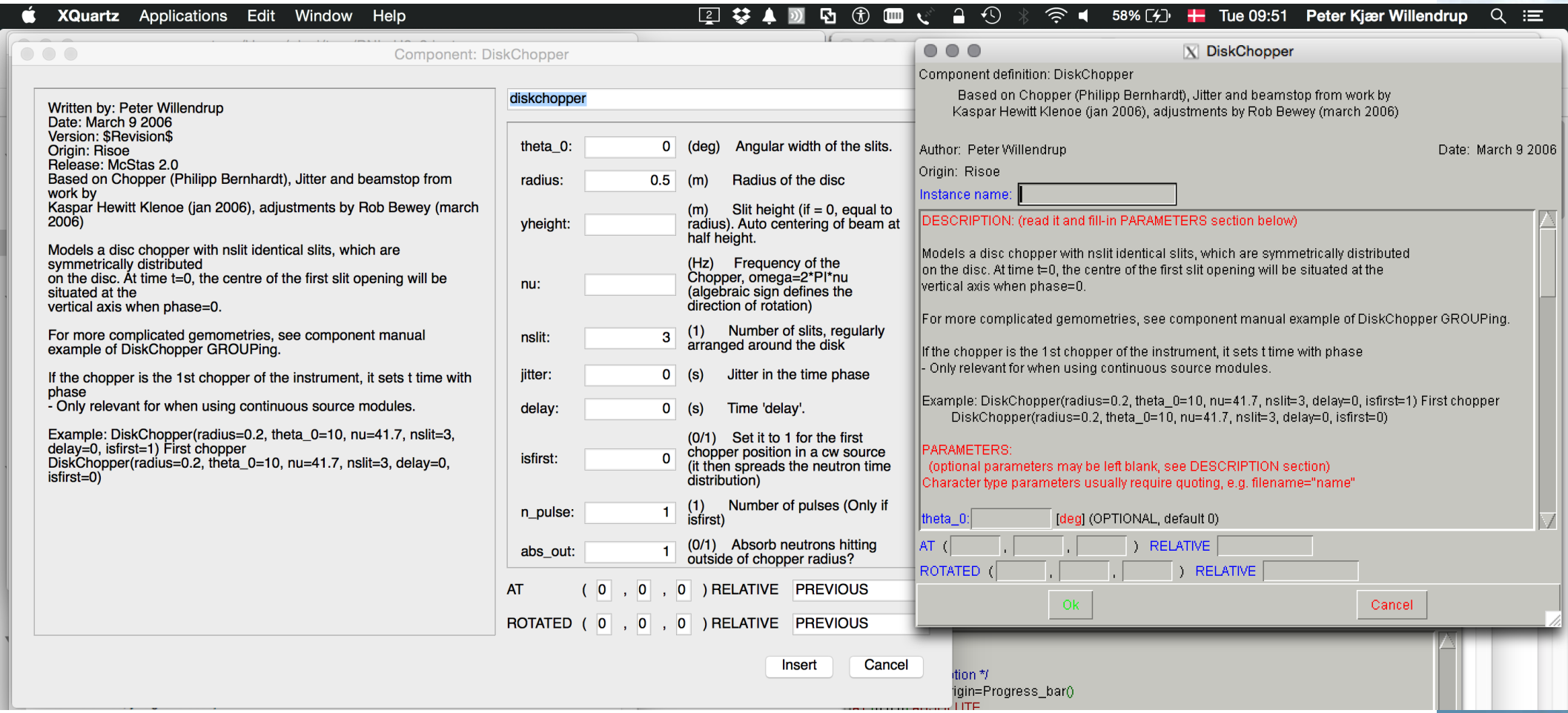
mcgui - pl vs py versions



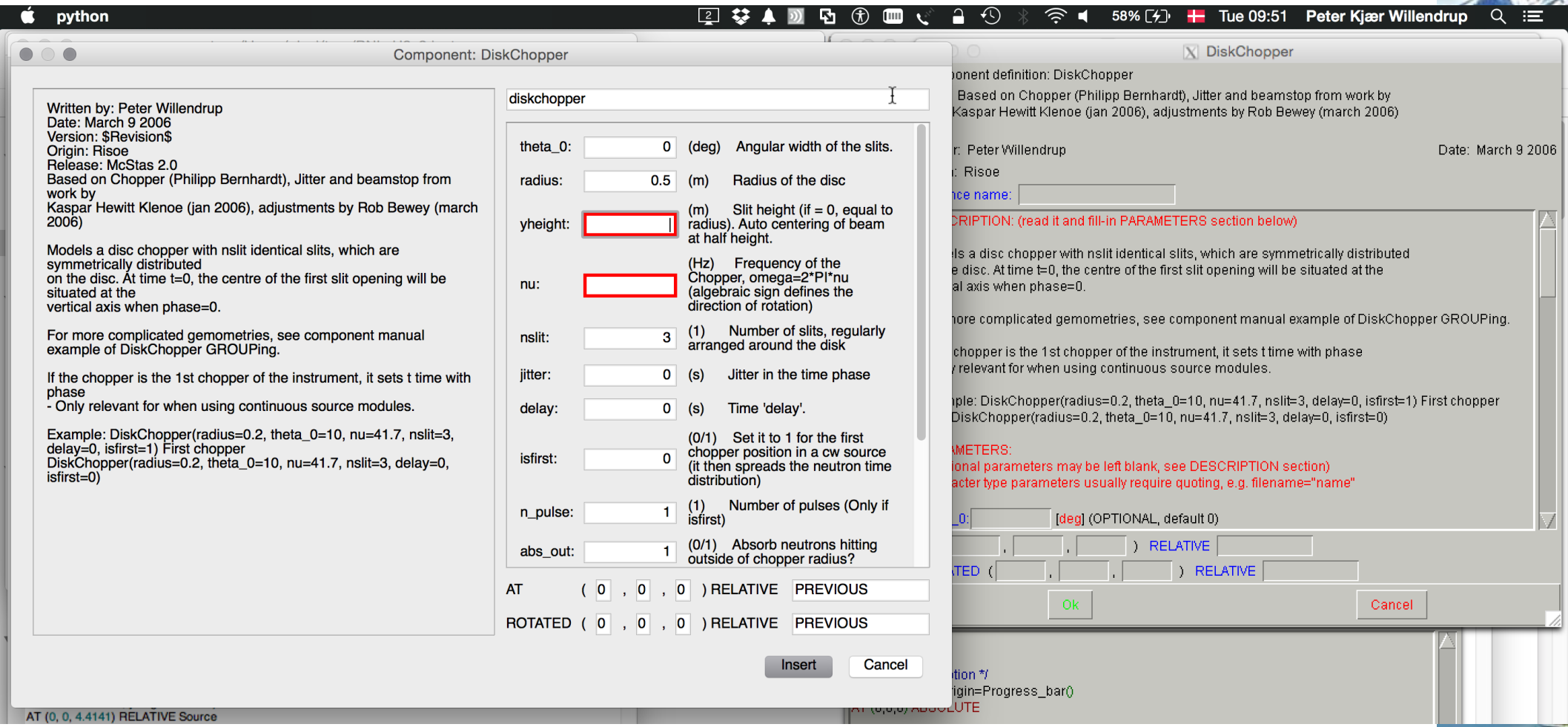
```
TRACE
/* Source description */
COMPONENT Origin=Progress_bar()
AT (0,0,0) ABSOLUTE

/* 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, 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,
```

```
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, 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, 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
```

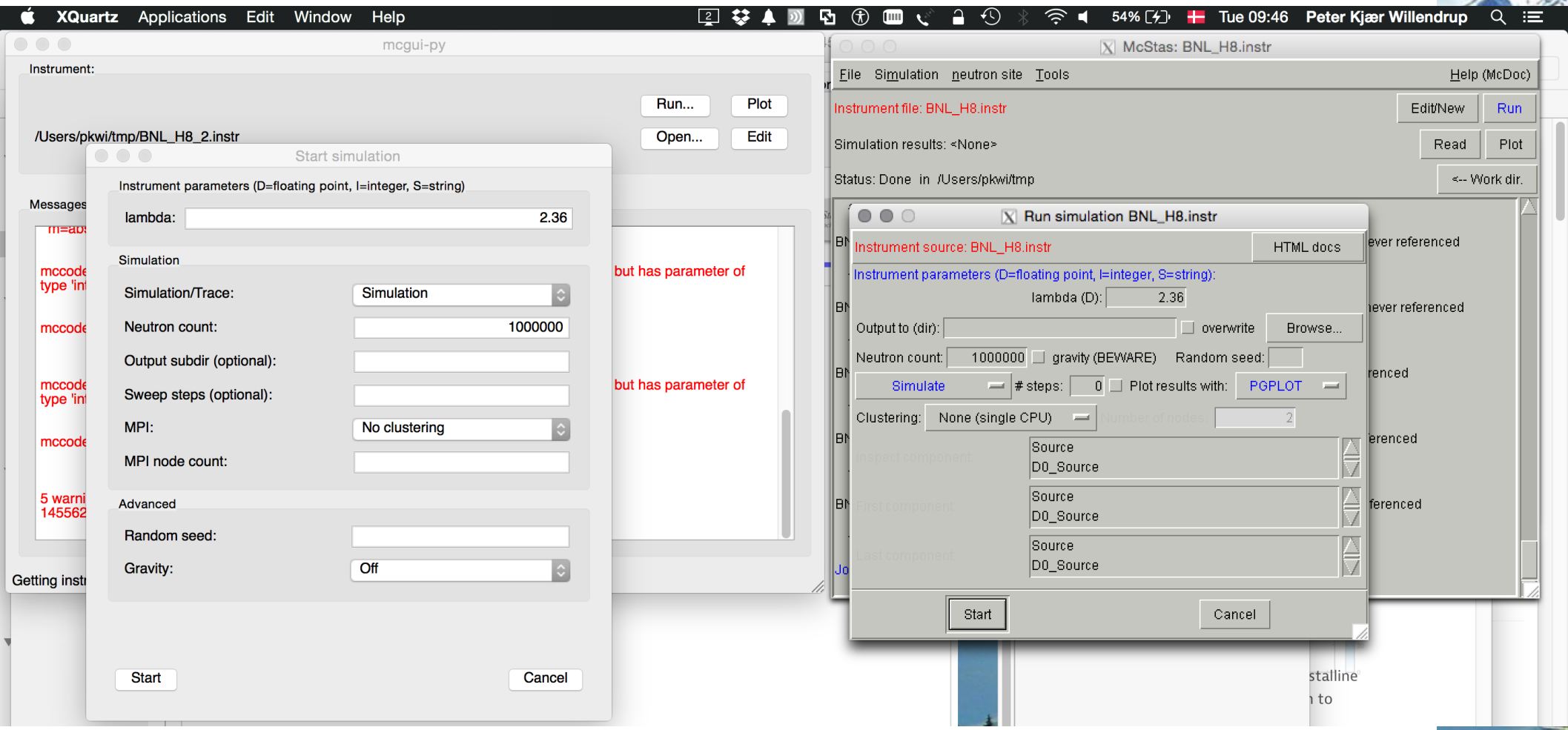
mcgui - pl vs py versions



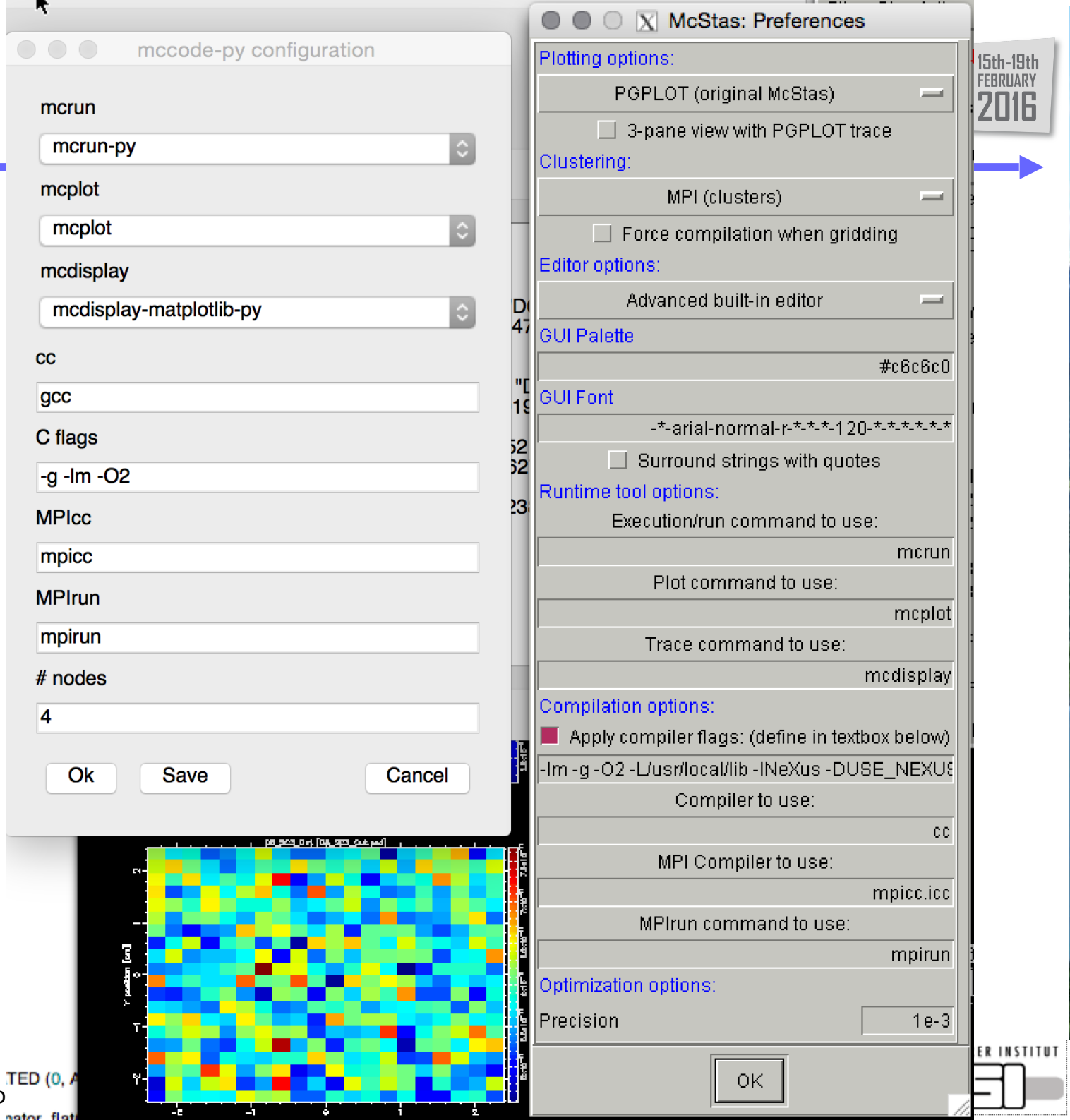
mcgui - pl vs py versions



mcgui - pl vs py versions



mcgui -


mccode-py configuration
mcrun
mcrun-py
mcplot
mcplot
mcdisplay
mcdisplay-matplotlib-py
cc
gcc
C flags
-g -lm -O2
MPIcc
mpicc
MPIrun
mpirun
nodes
4
Ok
Save
Cancel
McStas: Preferences
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)
-lm -g -O2 -L/usr/local/lib -INeXus -DUSE_NEXUS
Compiler to use:
cc
MPI Compiler to use:
mpicc.icc
MPIrun command to use:
mpirun
Optimization options:
Precision
1e-3
OK
15th-19th
FEBRUARY
2016

mcrun pl vs py versions

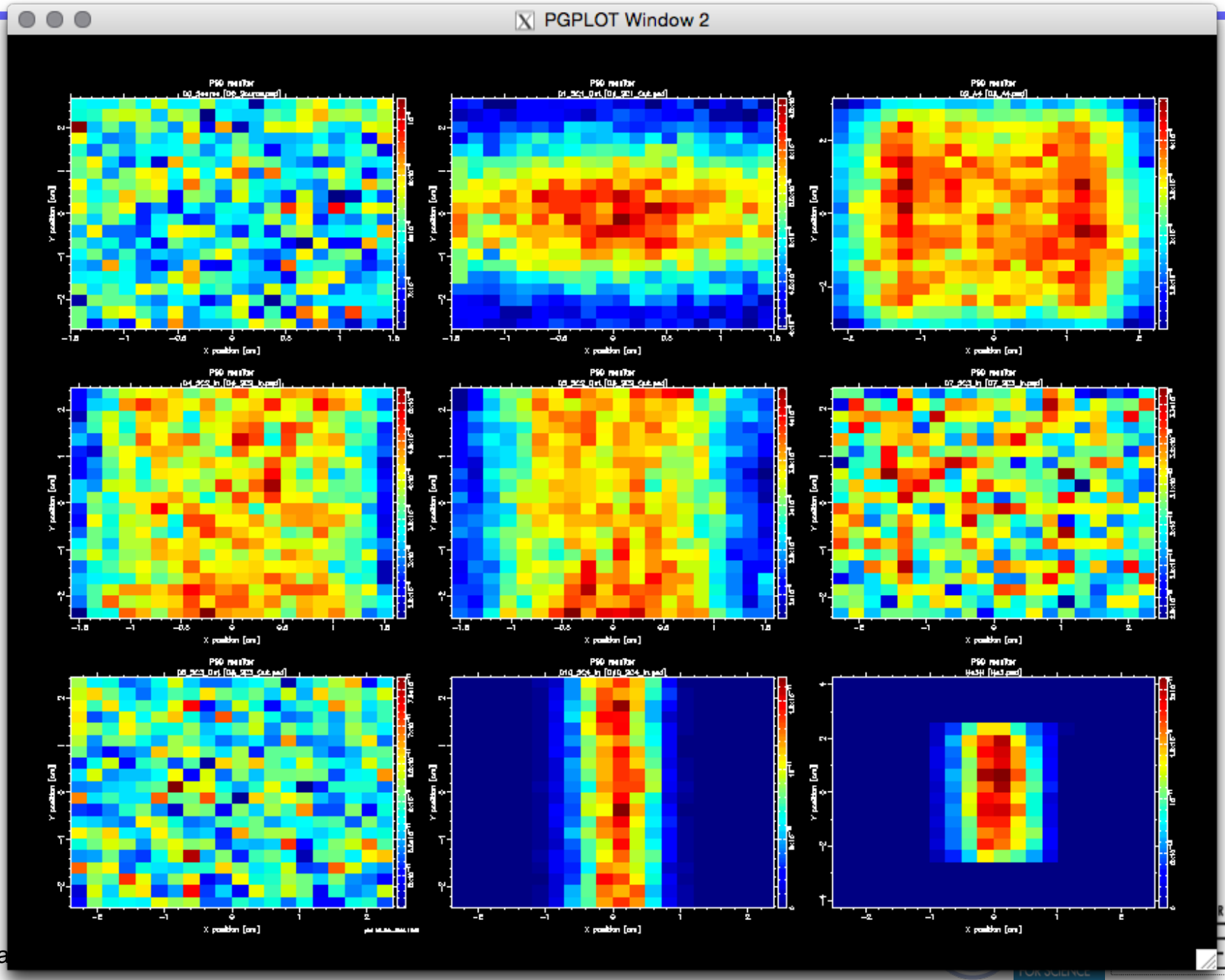
tmp — pkwi@pkwi-mbp15: ~/tmp — bash — 88×50

```
XQuartzScreenSnapz004.png
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 [-sndftgahi] 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=NB_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$
```

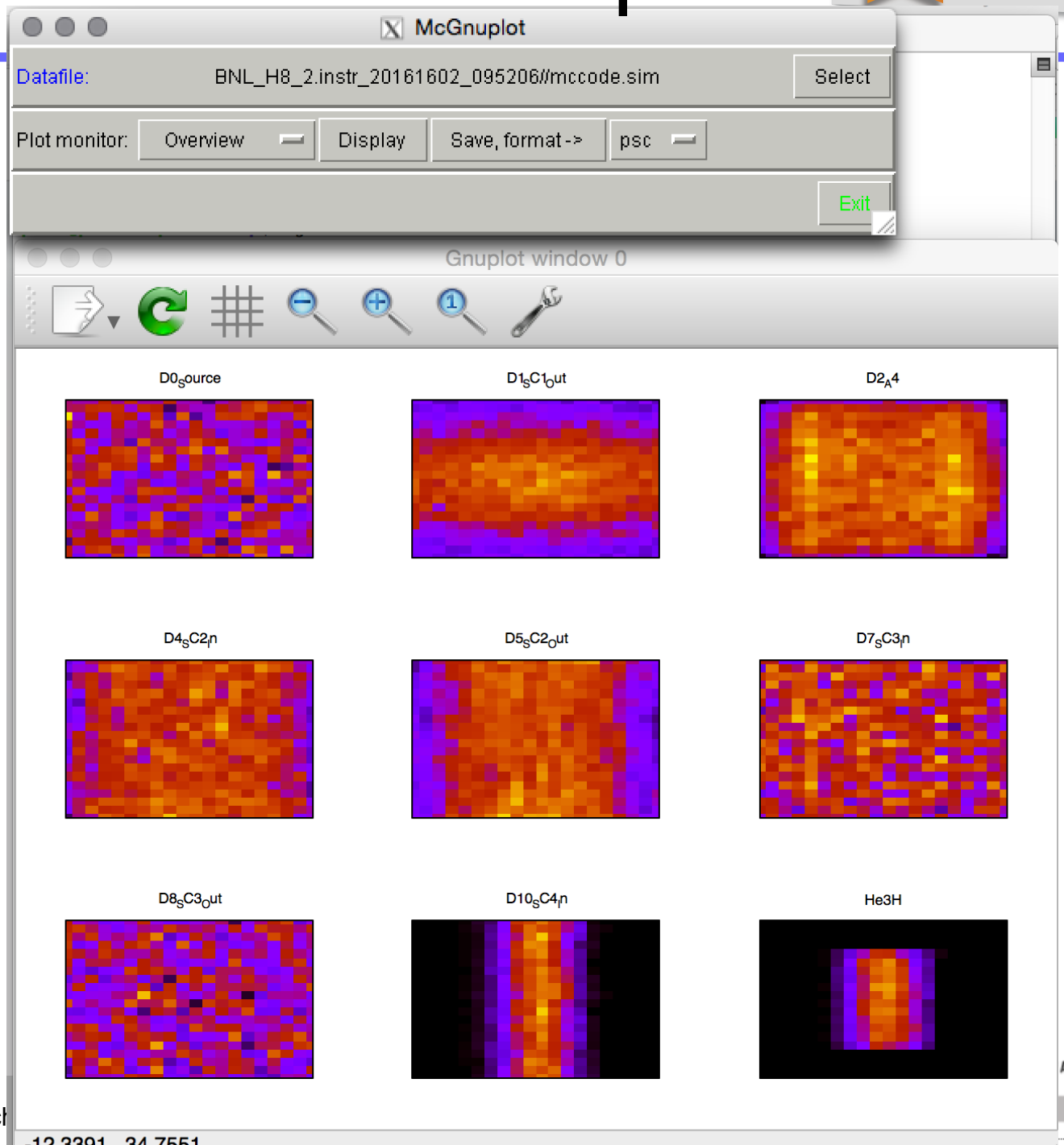
tmp — pkwi@pkwi-mbp15: ~/tmp — bash — 103×49

```
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 [-sndftgahi] 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=NB_CPU    Spawn simulations to multiple machine/cores grid.
             --multi=NB_CPU     see the documentation for more info.
   --mpi     --mpi=NB_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                    Maximize 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$
```

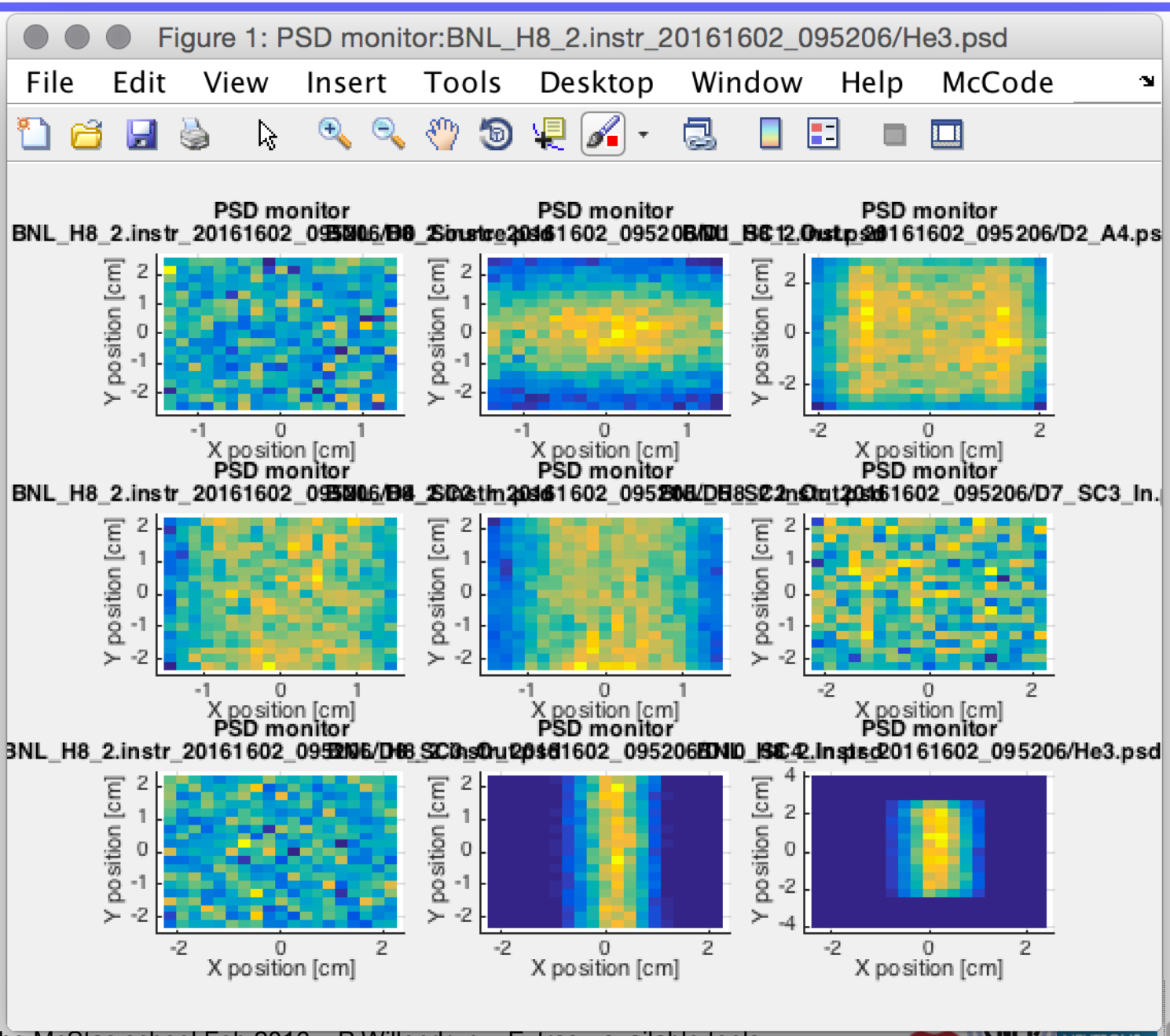
mcplot (--format=PGPLOT)



mcplot --format=Gnuplot



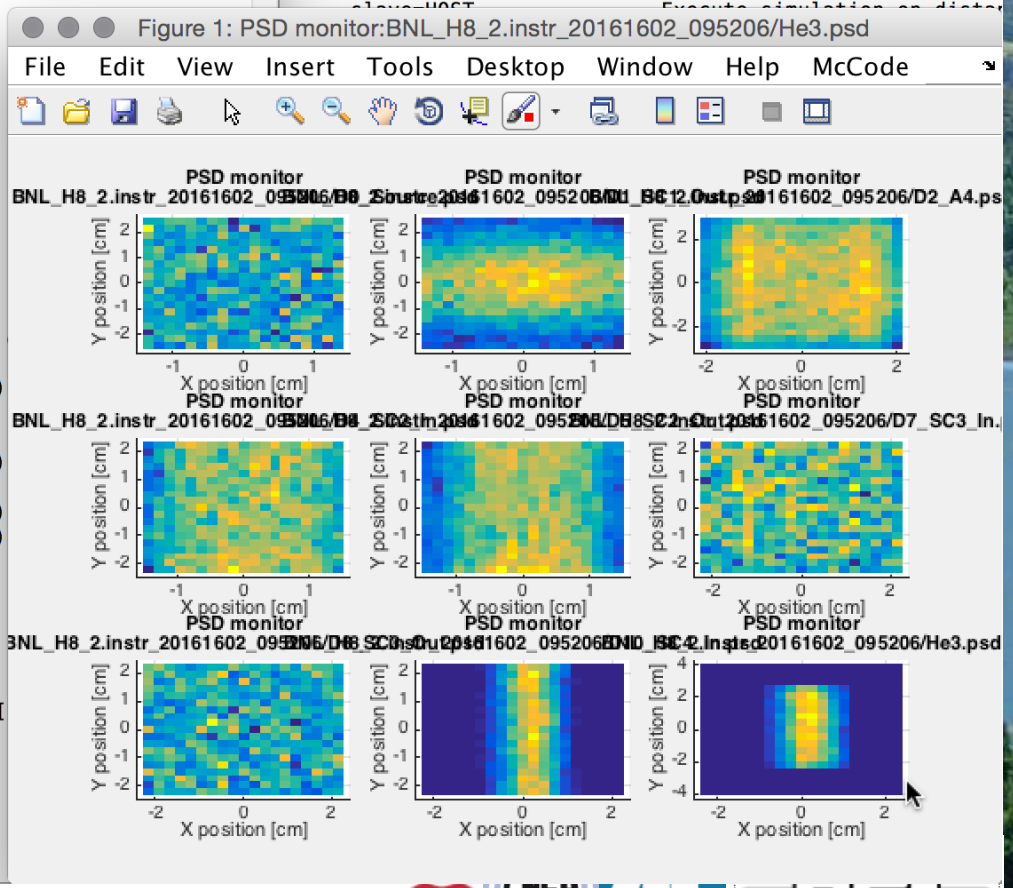
mcplot --format=Matlab



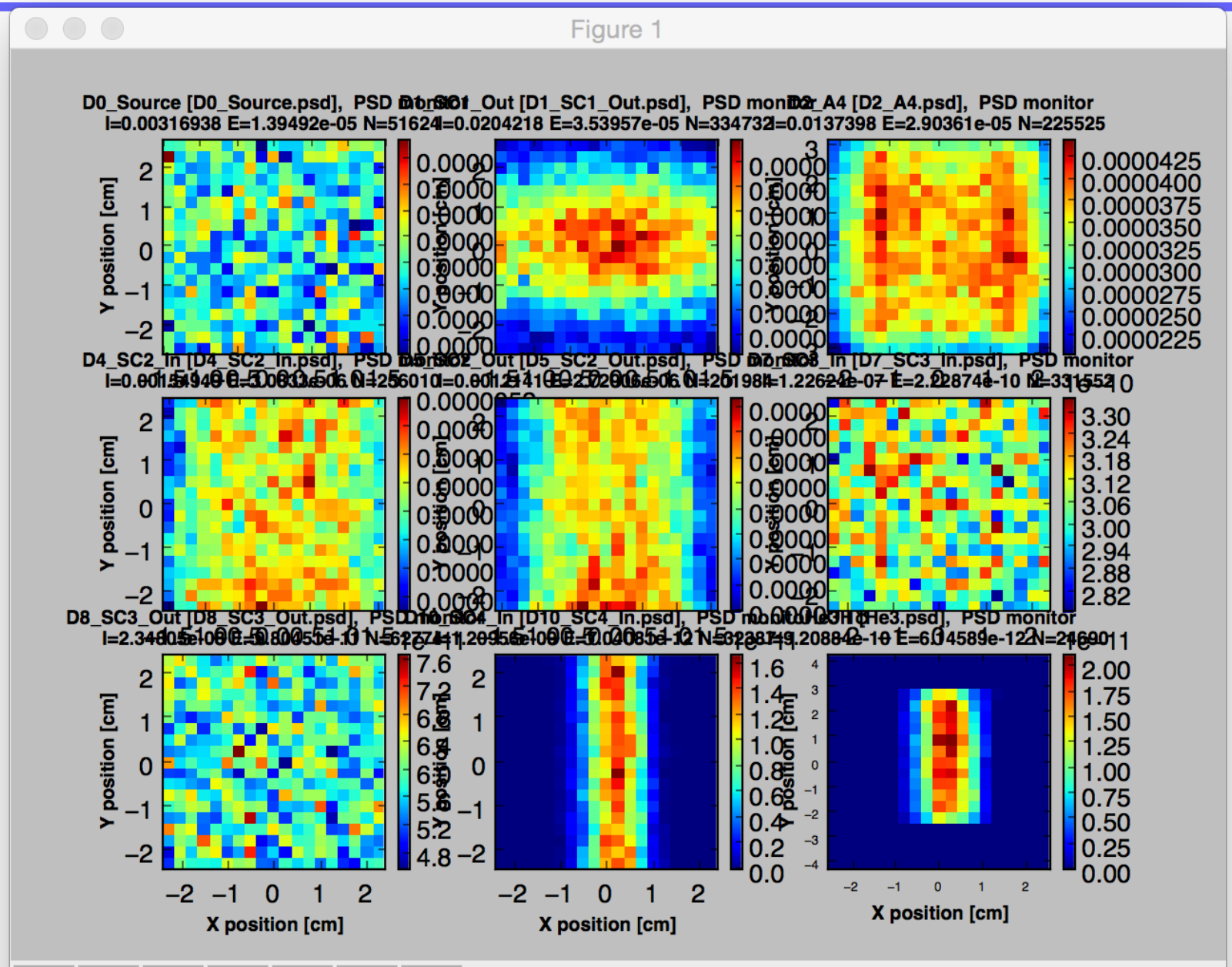
mcplot-matlab


```
tmp — pkwi@pkwi-mbp15: ~/tmp — MATLAB — 88×50
/usr/local/bin/mcplot: reading local mcstas configuration from /Users/pkwi/.mcstas/mccod
e_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
^C
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) >
                  Copyright 1984-2014 The MathWorks, Inc.
                   R2014b (8.4.0.150421) 64-bit (maci64)
                             September 15, 2014


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]

>>
```

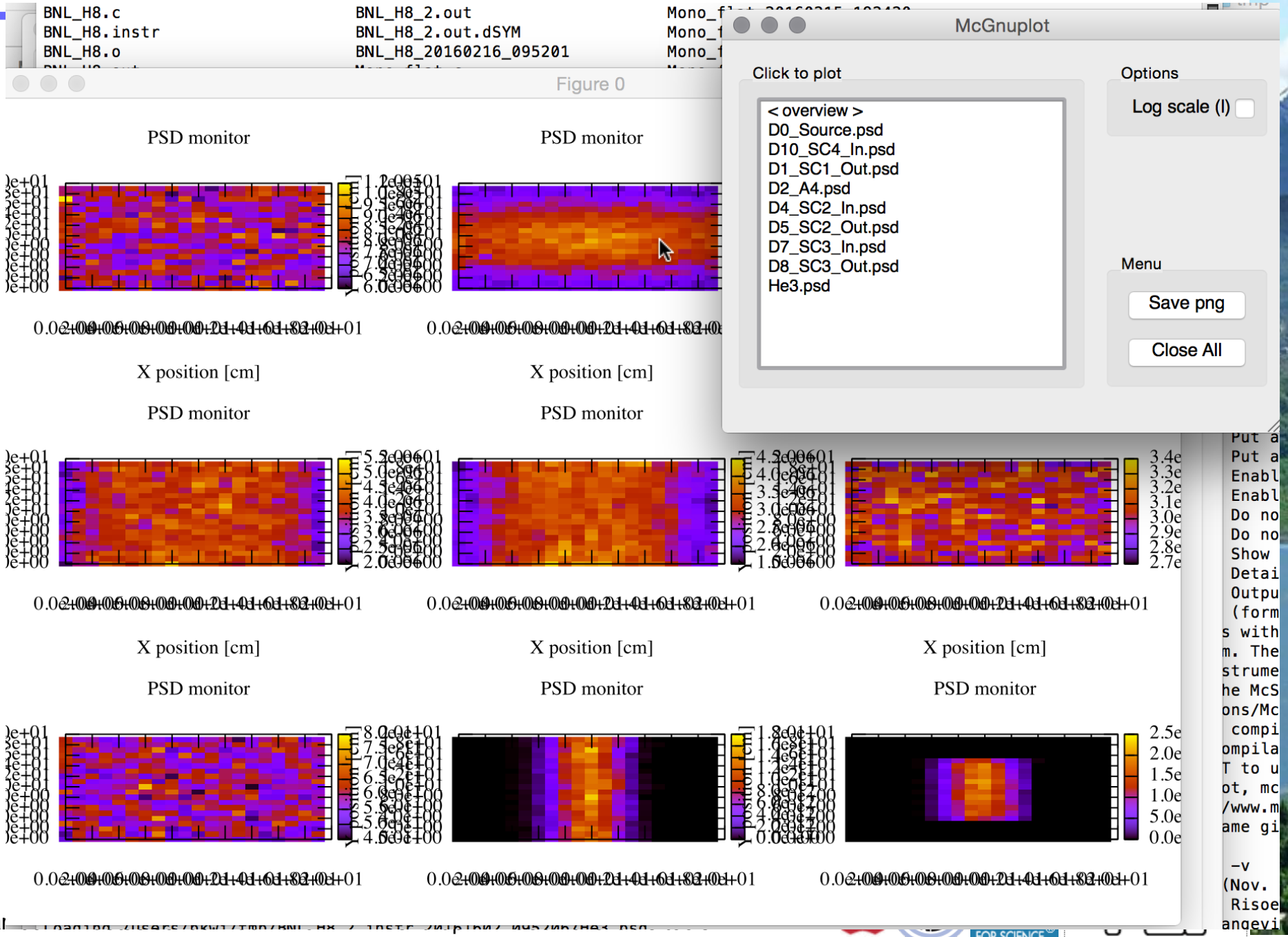
```
tmp — pkwi@pkwi-mbp15: ~/t
pkwi@pkwi-mbp15:~/tmp$ mcrun --help
mcrun: reading local mcstas configuration from /Users/pkw
/usr/local/bin/mcrun: reading local mcstas configuration
*** No directory given - placing data in _20160216_095914
"Usage: mcrun [-cpnN] Instr [-sndftgahi] params={val|min,
mcrun options:
   -c        --force-compile  Force rebuilding of instrume
   -p FILE   --param=FILE     Read parameters from file F
   -n COUNT  --ncount=COUNT   Set number of neutrons to s
   -N NP     --numpoints=NP   Set number of scan points.
             --grid=NB_CPU    Spawn simulations to multip
             --multi=NB_CPU     see the documentation for
   --mpi     --mpi=NB_CPU     Spread simulation over NB_CP
   --machines=MACHINES        Read machine names from file
```



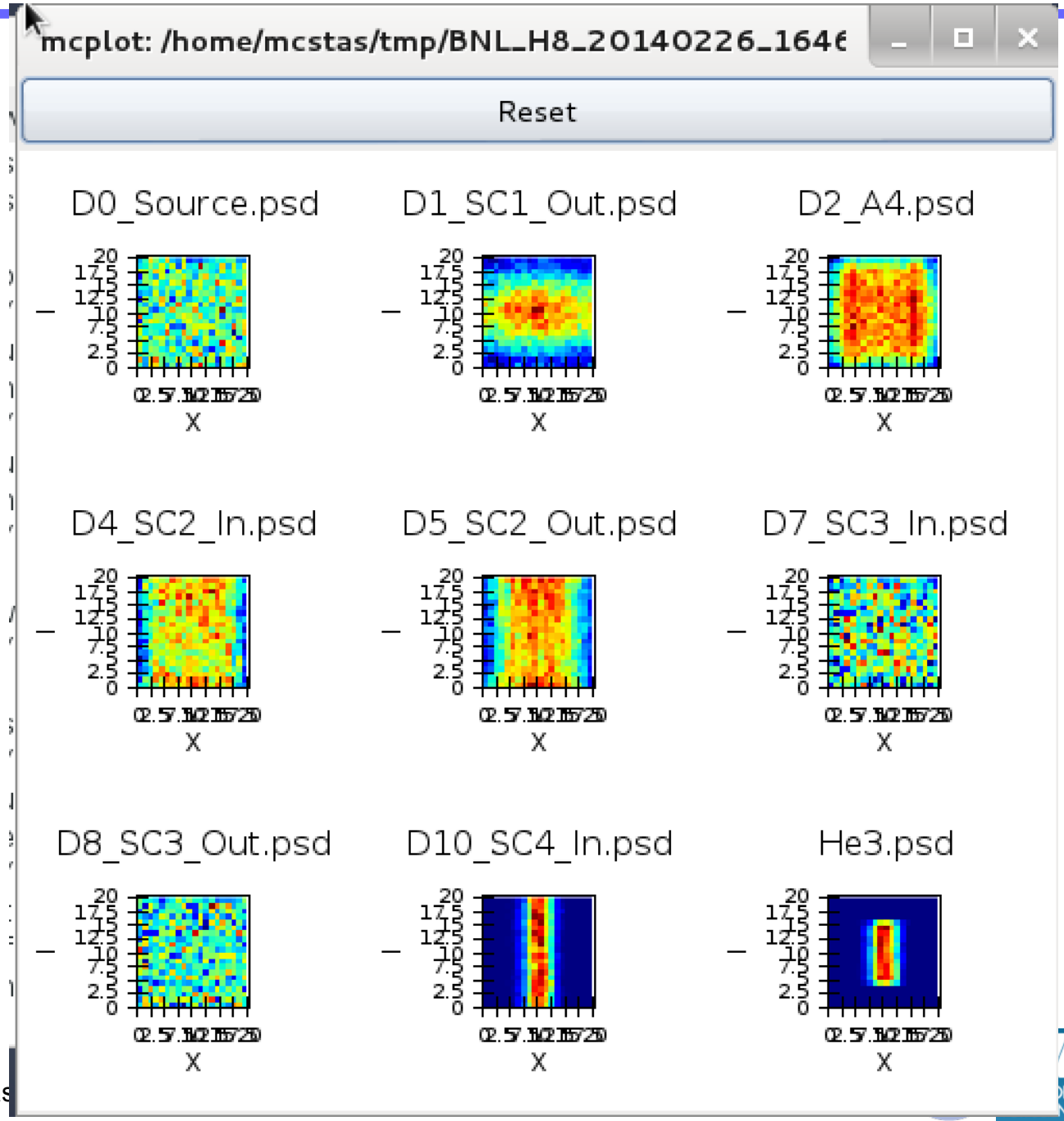
mcplot-matplotlib-py



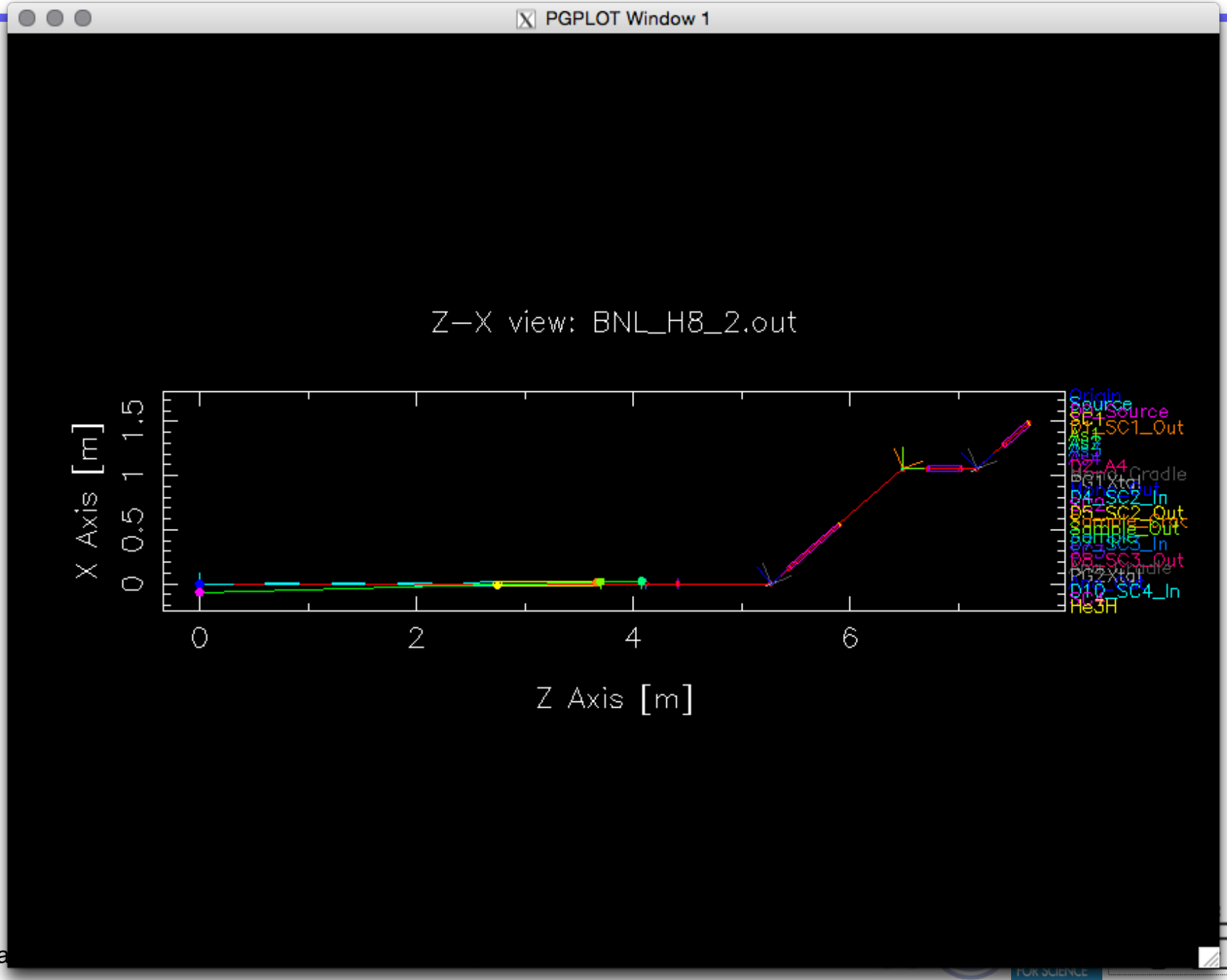
mcplot-gnuplot-py



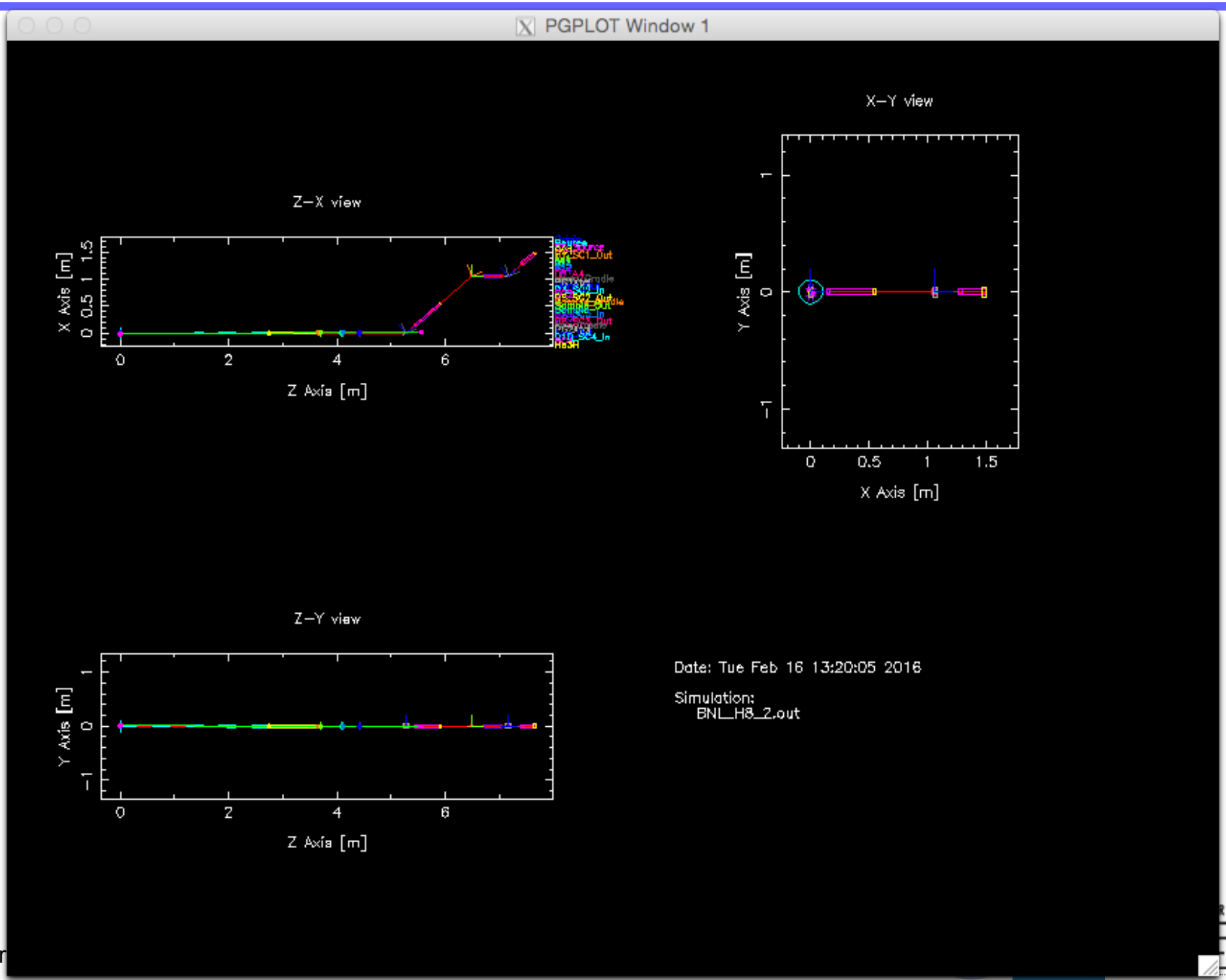
mcplot-chaco-py



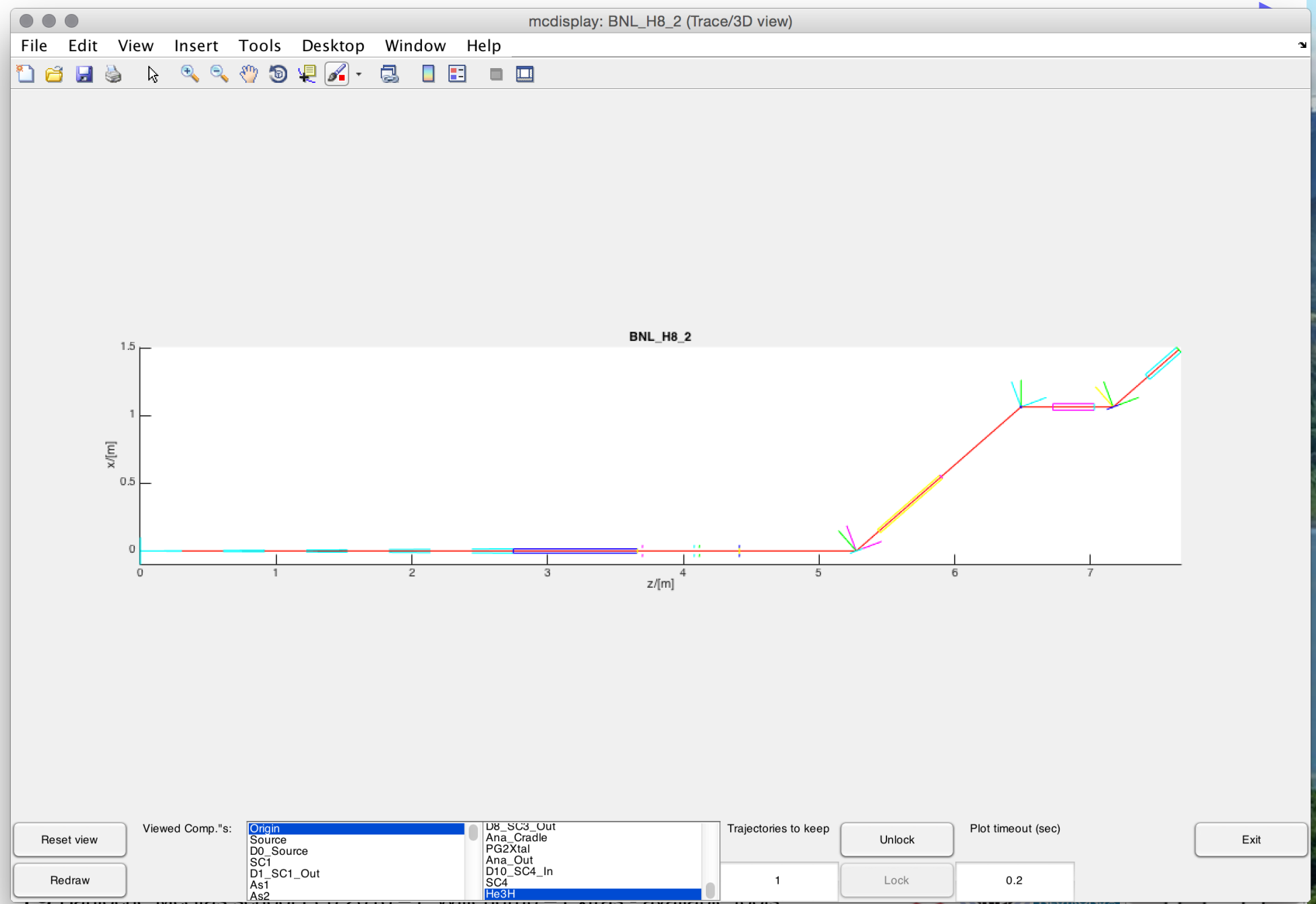
mcdisplay


PGPLOT Window 1
Z–X view: BNL_H8_2.out
X Axis [m]
0 0.5 1 1.5
0
2
4
6
Z Axis [m]
Origin
Source
SC1_Out
A4
Gradle
Xtal
SC2_In
SC2_Out
SC3_In
SC3_Out
SC4_In
He3H

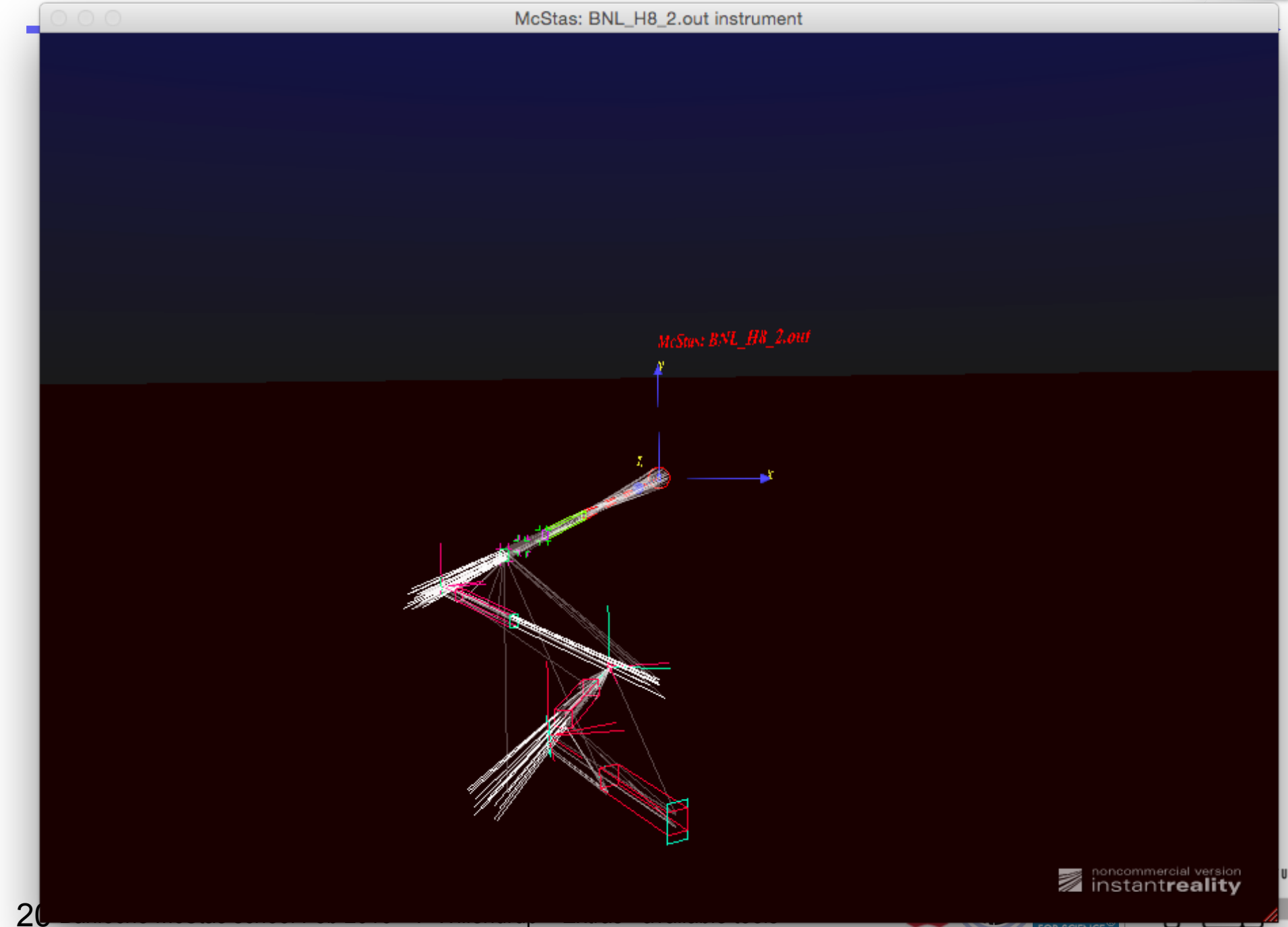
mcdisplay -m


PGPLOT Window 1
Z–X view
X Axis [m]
Z Axis [m]
X–Y view
Y Axis [m]
X Axis [m]
Z–Y view
Y Axis [m]
Z Axis [m]
Date: Tue Feb 16 13:20:05 2016
Simulation:
BNL_H8_2.out

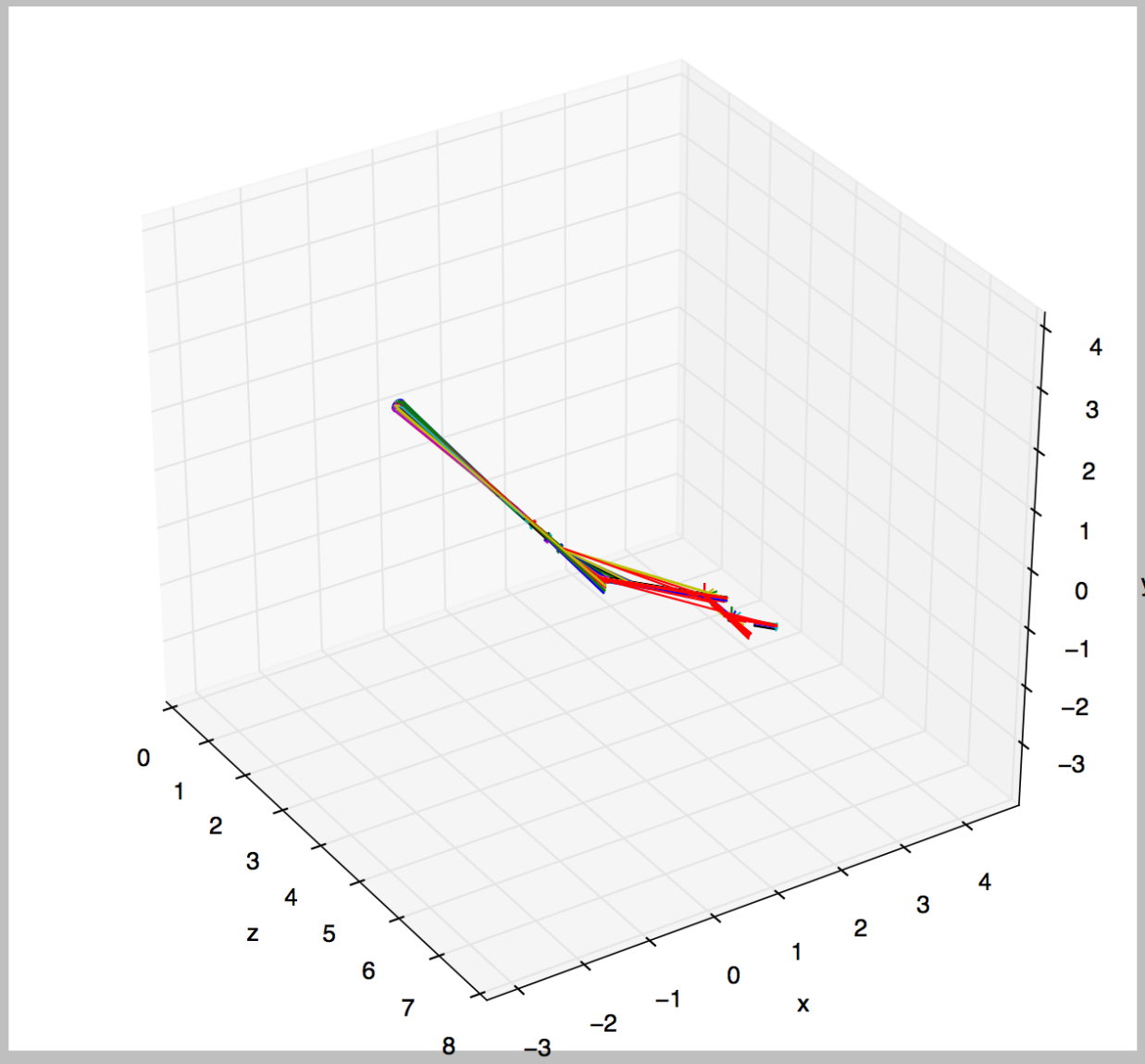
mcdisplay --format=Matlab



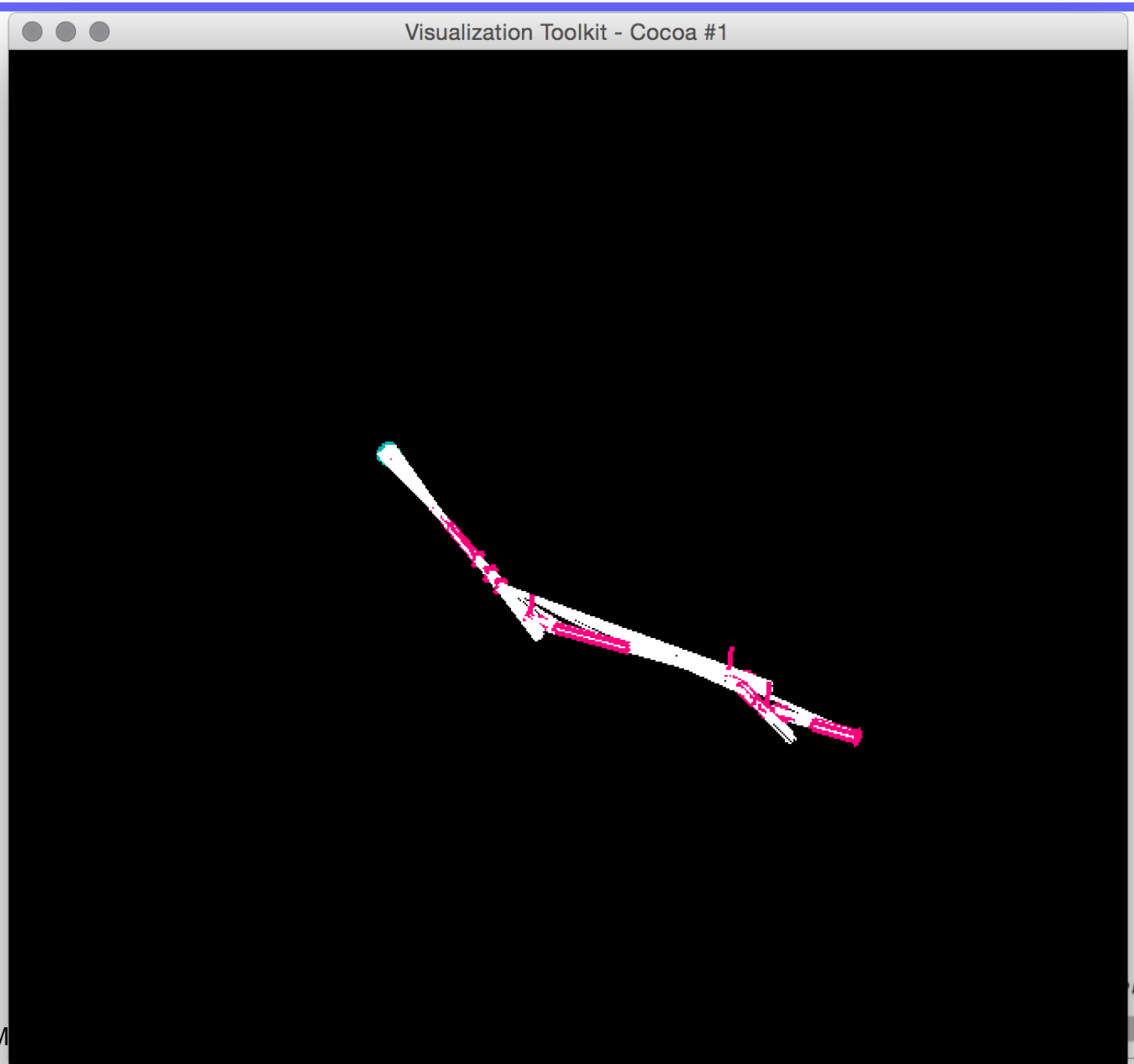
mcdisplay --format=VRML



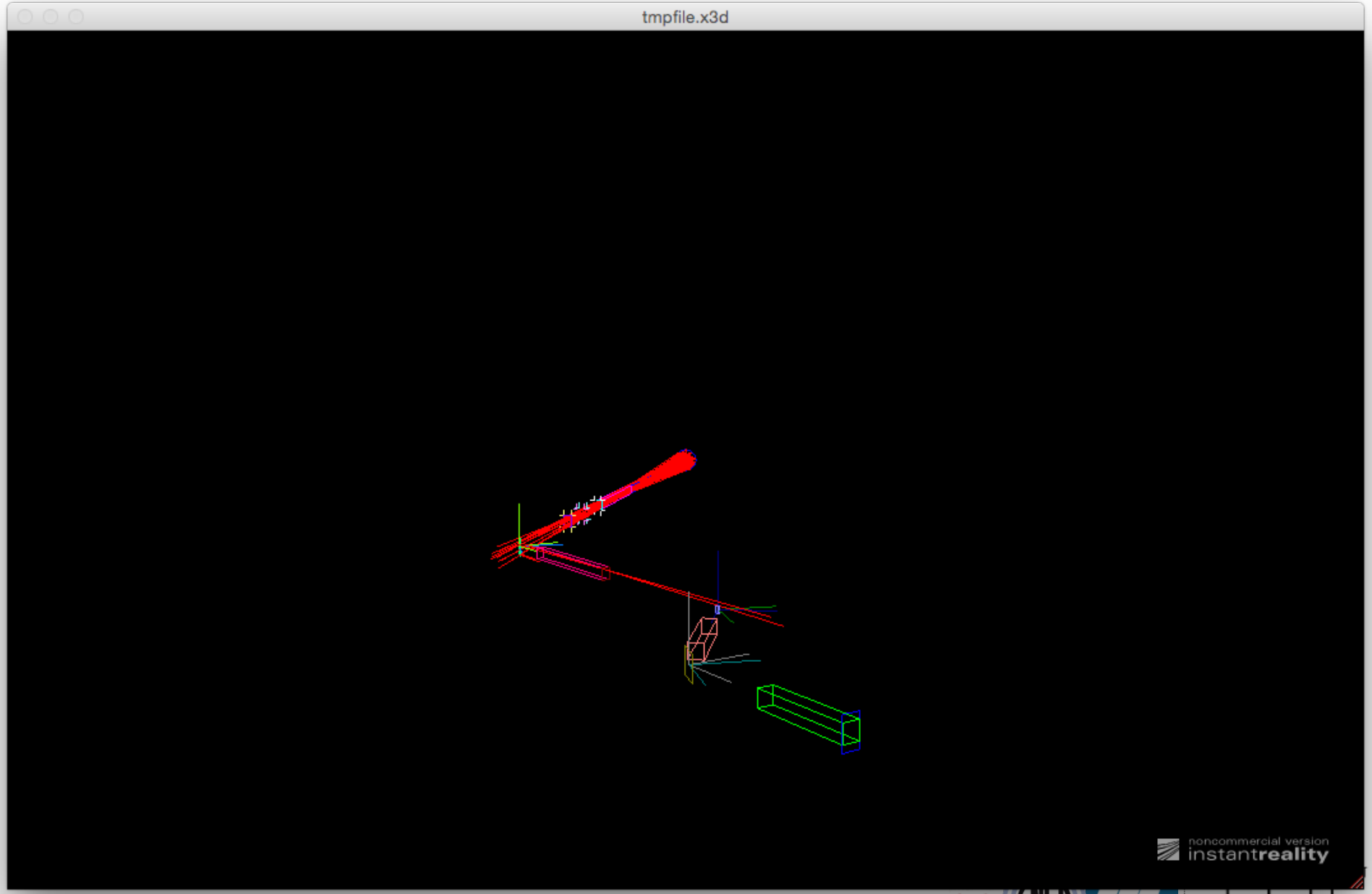
mcdisplay-matplotlib-py



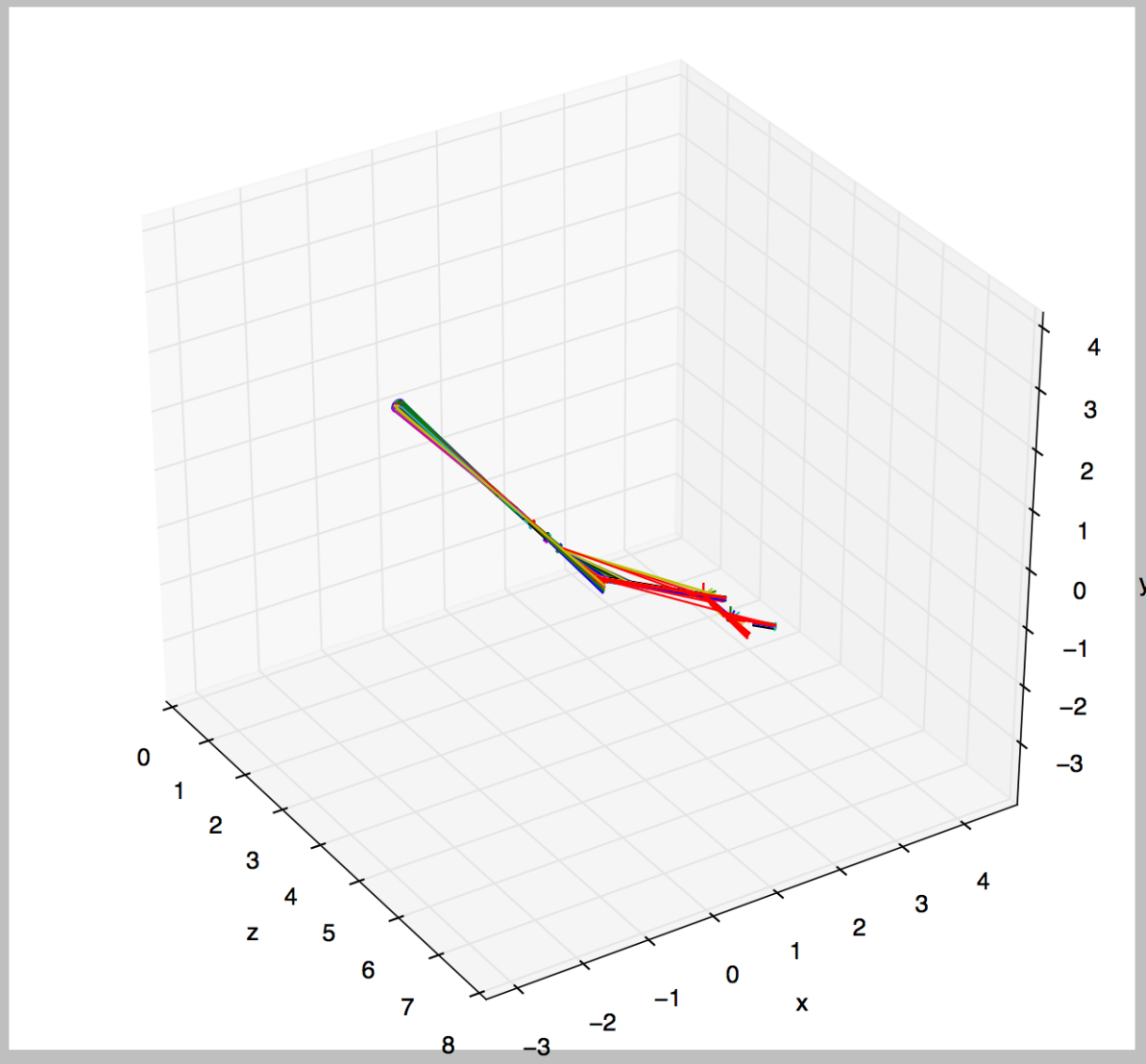
mcdisplay-vtk-py



mcdisplay-x3d-py



mcdisplay --format=VRML



Web interface @ e-neutrons.org

sim.e-neutrons.org

Apple Remote ... (kickstart) SpinW Software for...el Computers Studerende sø...| Dikutal.dk Bachmann N ...4896 | eBay Bachmann Tra...uct Catalog

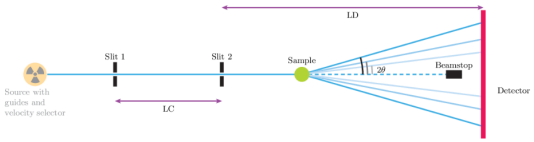
Instrument

McStas

e-neutrons

Logged in as pwillendrup (see recent simruns) Logout

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 – 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.

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sim.e-neutrons.org

Apple Remote ... (kickstart) SpinW Software for...el Computers Studerende sø...| Dikutal.dk Bachmann N ...4896 | eBay Bachmann Tra...uct Catalog

Simulation Data

SANSsimple

Completed 15:57:50, 16/12-2015

Reconfigure

Simulation

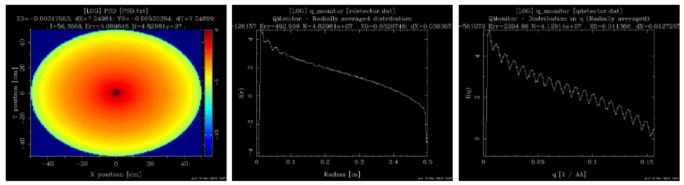
params: pinhole_rad=0.004 LC=3 LD=3 Lambda=6 DLambda=0.6 R=400 dR=0 dbilayer=35 PHI=0.01 Delta_Rho=0.6 Qmax=0.3 BEAMSTOP=1 SAMPLE=1

neutron rays: 10000000

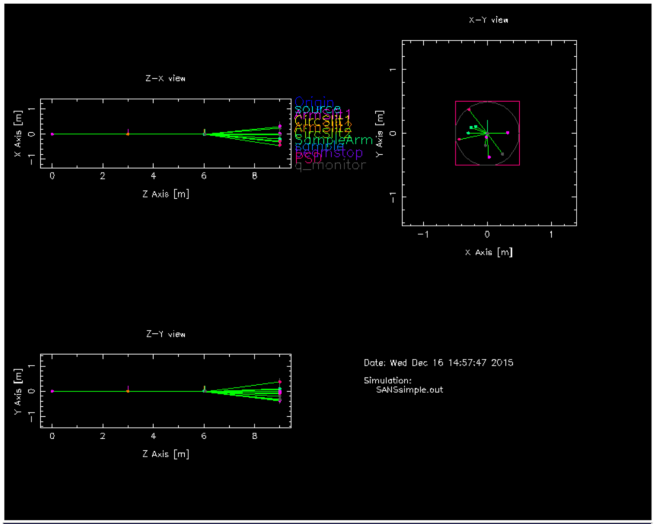
random seed: 0

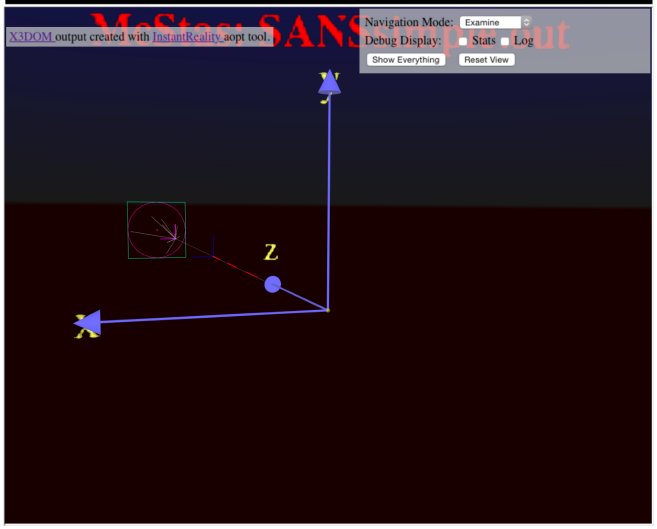
simulation steps: 1

Data plots (click here for lin-scale)



Instrument layout





Web interface @ e-neutrons.org

sim.e-neutrons.org

Apple Remote ... (kickstart) SpinW Software for...el Computers Studerende sø...| Dikutal.dk Bachmann N ...4896 | eBay Bachmann Tra...uct Catalog

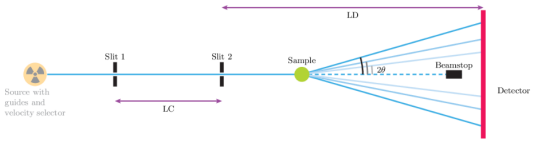
Instrument

McStas

e-neutrons

Logged in as pwillendrup (see recent simruns) Logout

SANSsimple (click for documentation)



Parameters for SANSsimple

pinhole_rad [m] :	0.004	radius of th
LC [m] :	3	length of t
LD [m] :	3	distance be
Lambda [Angs] :	6	Average wa
DLambda [Angs] :	0.6	Wavelengt
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.

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Only pre-defined instruments!!!

sim.e-neutrons.org

Simulation Data

SANSsimple

Completed 15:57:50, 16/12-2015

Reconfigure

Simulation

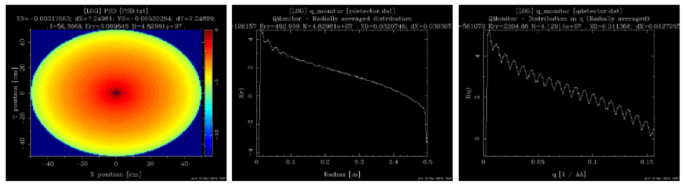
params: pinhole_rad=0.004 LC=3 LD=3 Lambda=6 DLambda=0.6 R=400 dR=0 dbilayer=35 PHI=0.01 Delta_Rho=0.6 Qmax=0.3 BEAMSTOP=1 SAMPLE=1

neutron rays: 10000000

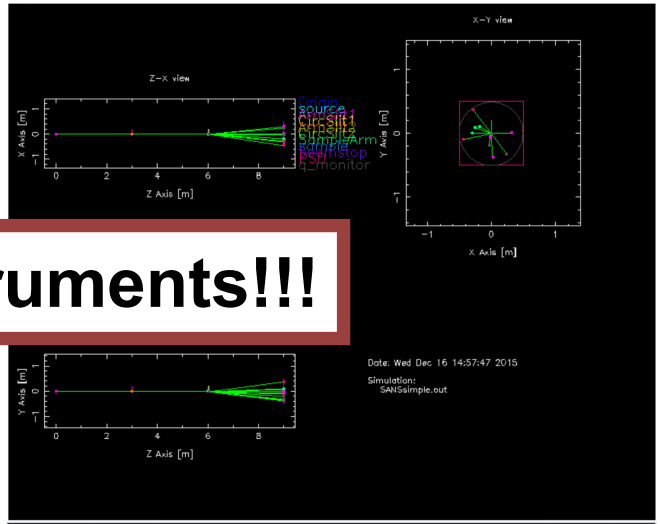
random seed: 0

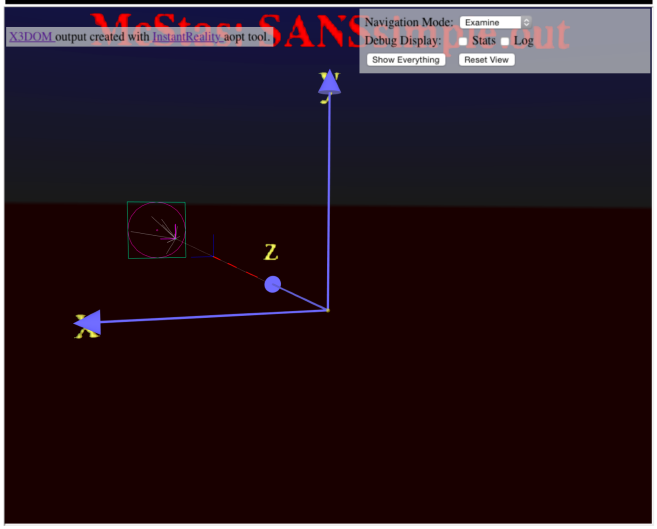
simulation steps: 1

Data plots (click here for lin-scale)

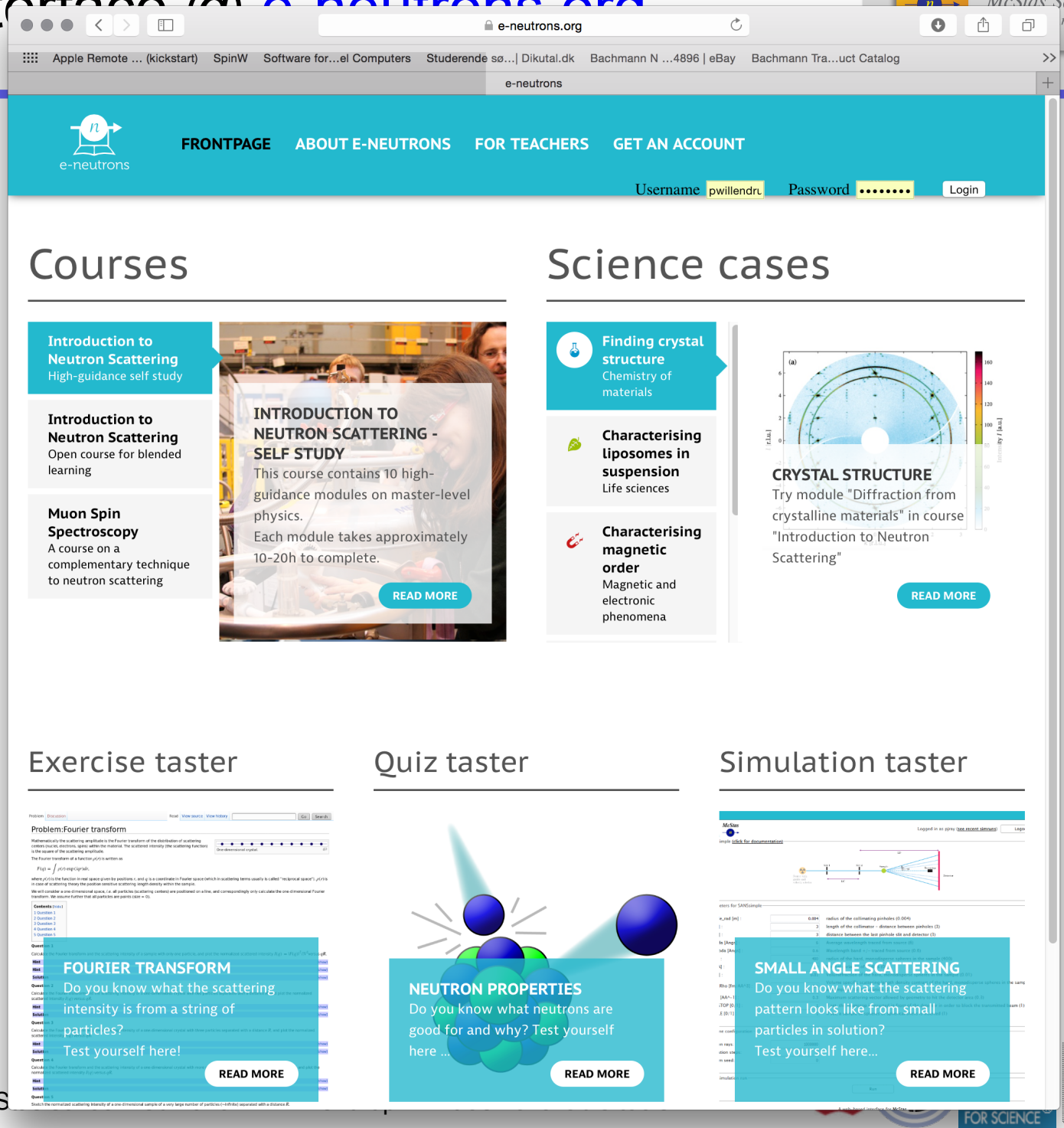


Instrument layout

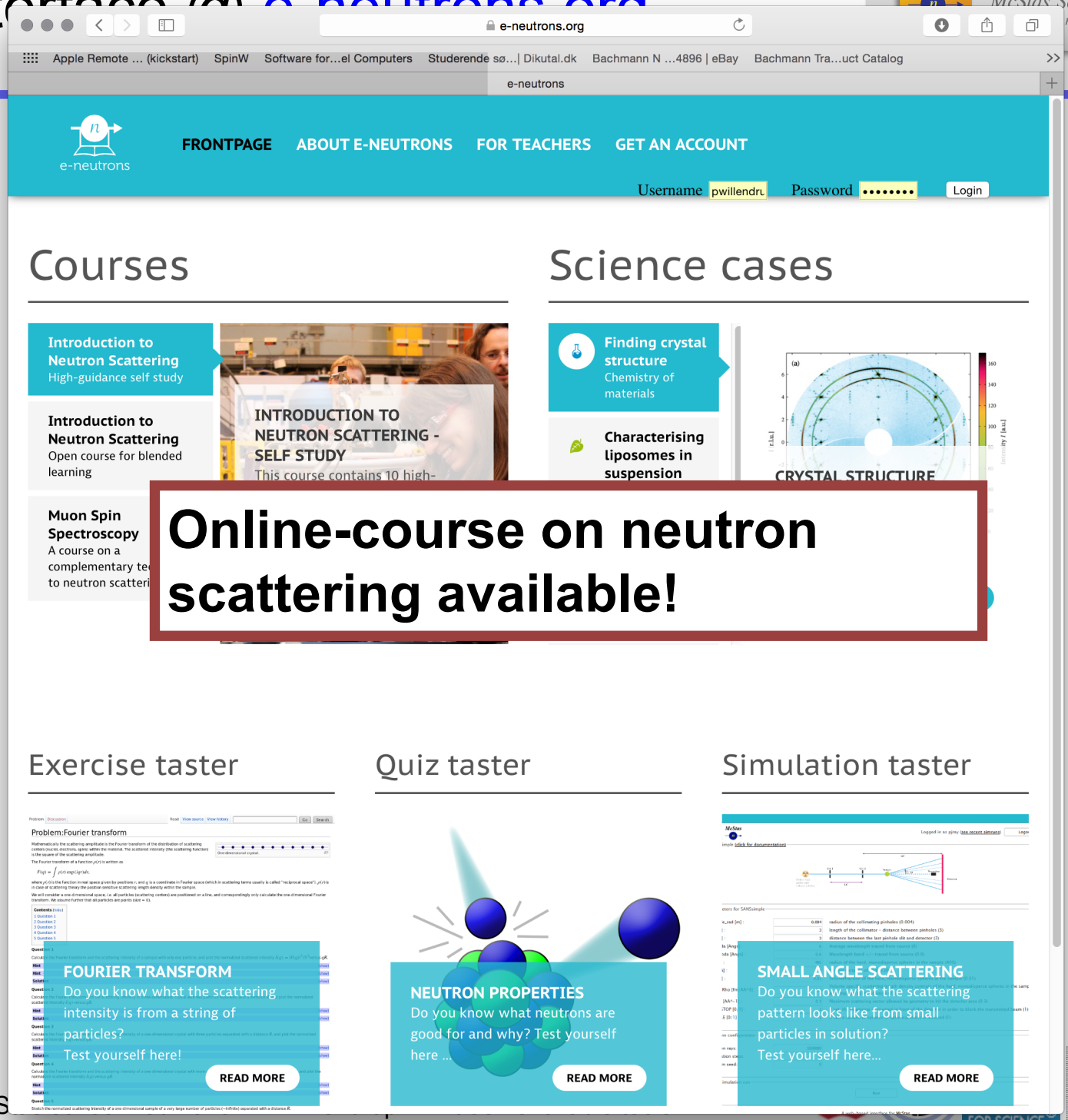




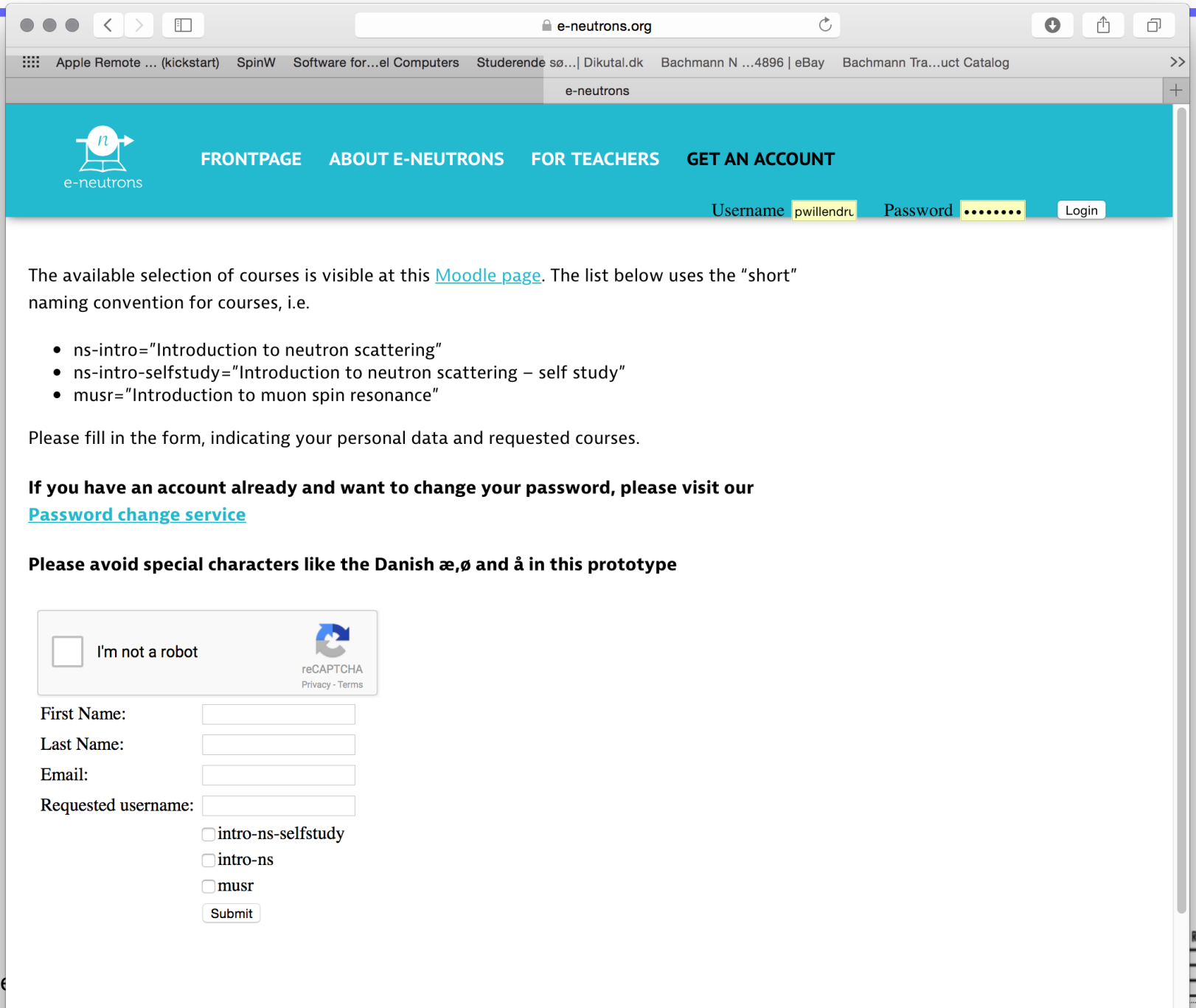
Web interface @ e-neutrons.org



Web interface @ e-neutrons.org



Web interface @ e-neutrons.org



Web interface @ e-neutrons.org