

New features in McStas 2.4



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Agenda

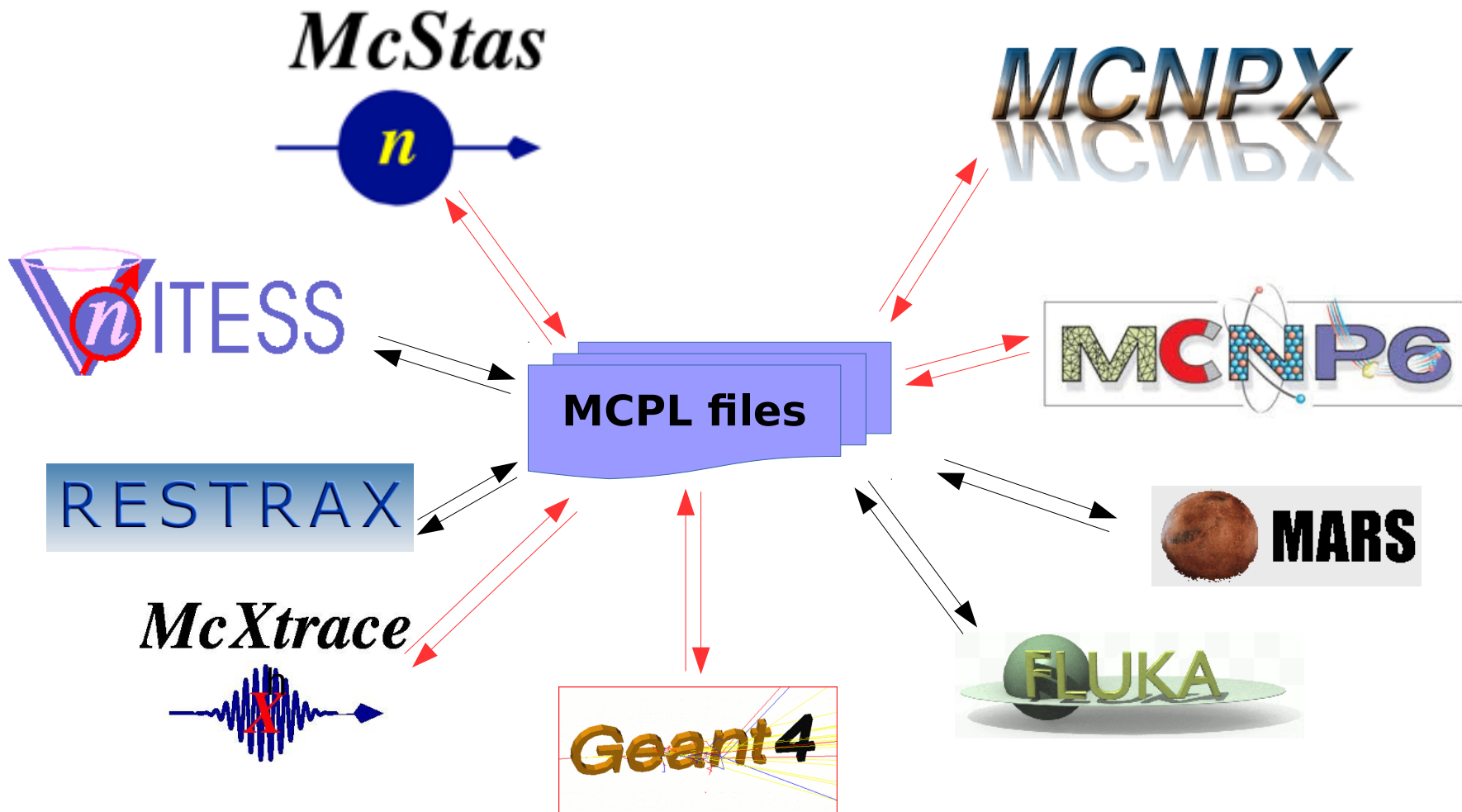
- Highlighted new features in 2.3 (April 2016) and 2.4 (May 2017)
 - Support for MCPL event files for interchange with e.g. Geant4 and MCNP
 - New component description of the ESS butterfly moderator
 - New user interface developments
 - The 'Union' component set for e.g. accurate description of complex sample environments



Improved MCPL support

The solution: A common interchange format.

MCPL: Monte Carlo Particle Lists



Improved MCPL support

The solution: A common interchange format.

MCPL: Monte Carlo Particle Lists

McStas

MCNPX

Further information:

- <https://mctools.github.io/mcpl/>
- <https://arxiv.org/abs/1609.02792>
- <http://coimbra2016.essworkshop.org>



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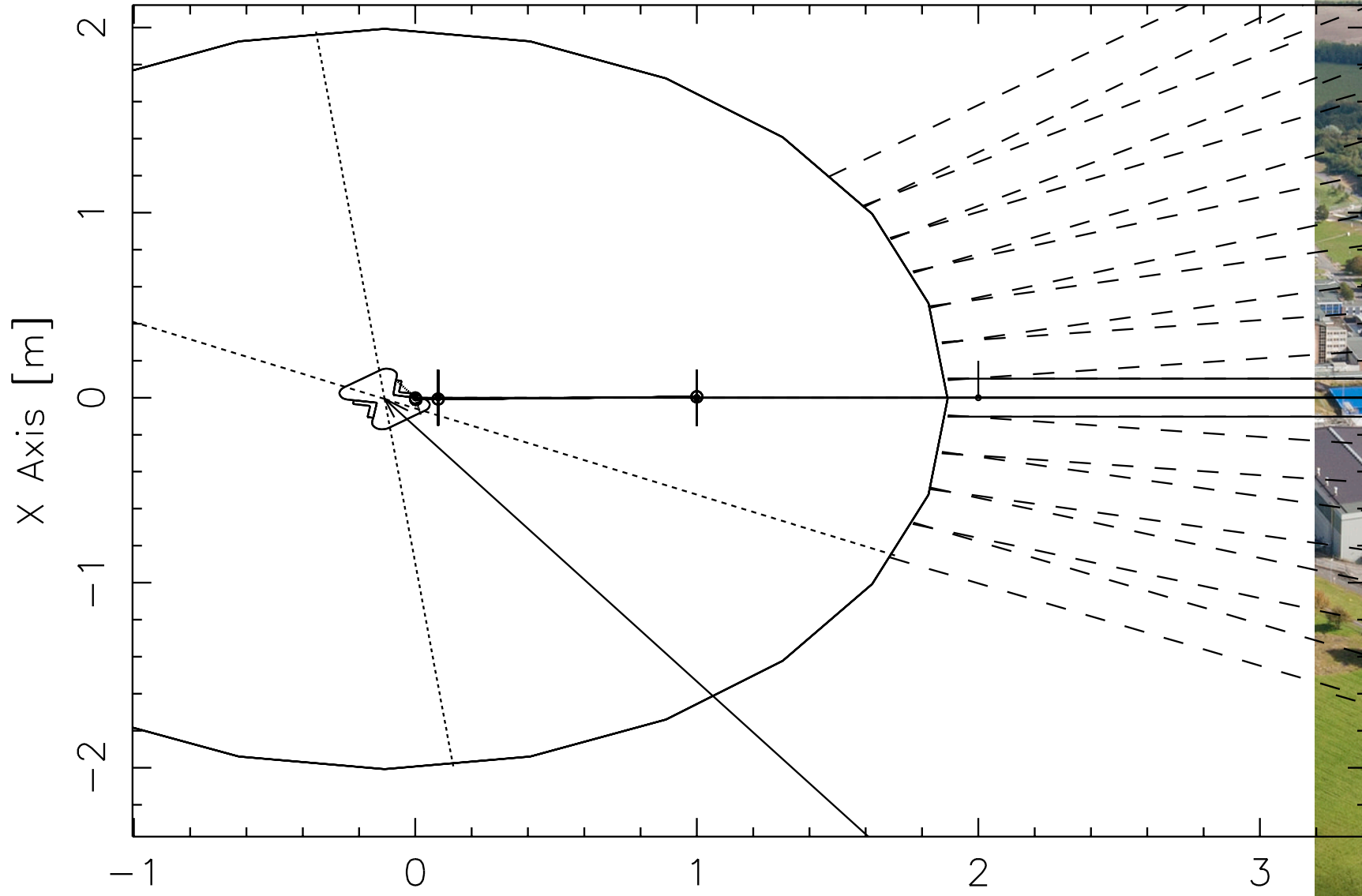


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ESS_butterfly mcdisplay output:

sector=N, beamline=5



ESS_butterfly McDoc page:

1. [Release document "Update to ESS Moderators, latest version"](#)
2. [Release document "Description and performance of the new baseline ESS moderators, latest version"](#)
3. http://ess_butterfly.mcstas.org/ benchmarking website with comparative McStas-MCNP figures
4. [html-based, interactive 3D model of moderators and monolith, as seen from beamline N4.](#)
5. [Source code](#) for ESS_butterfly.comp at GitHub.

Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
sector	str	Defines the 'sector' of your instrument position. Valid values are "N","S","E" and "W"	"N"
beamline	1	Defines the 'beamline number' of your instrument position. Valid values are 1..10 or 1..11 depending on sector	1
yheight	m	Defines the moderator height. Valid values are 0.03 m and 0.06 m	0.03
cold_frac	1	Defines the statistical fraction of events emitted from the cold part of the moderator	0.5
target_index	1	Relative index of component to focus at, e.g. next is +1 this is used to compute 'dist' automatically.	0
dist	m	Distance from origin to focusing rectangle; at (0,0,dist) - alternatively use target_index	0
focus_xw	m	Width of focusing rectangle	0
focus_yh	m	Height of focusing rectangle	0
c_performance	1	Cold brilliance scalar performance multiplier $c_performance > 0$	1
t_performance	1	Thermal brilliance scalar performance multiplier $t_performance > 0$	1
Lmin	AA	Minimum wavelength simulated	
Lmax	AA	Maximum wavelength simulated	
tmax_multiplier	1	Defined maximum emission time at moderator, $tmax = tmax_multiplier * ESS_PULSE_DURATION$.	3
n_pulses	1	Number of pulses simulated. 0 and 1 creates one pulse.	1
acc_power	MW	Accelerator power in MW	5

- See also http://ess_butterfly.mcstas.org

ESS_butterfly mcdisplay output:

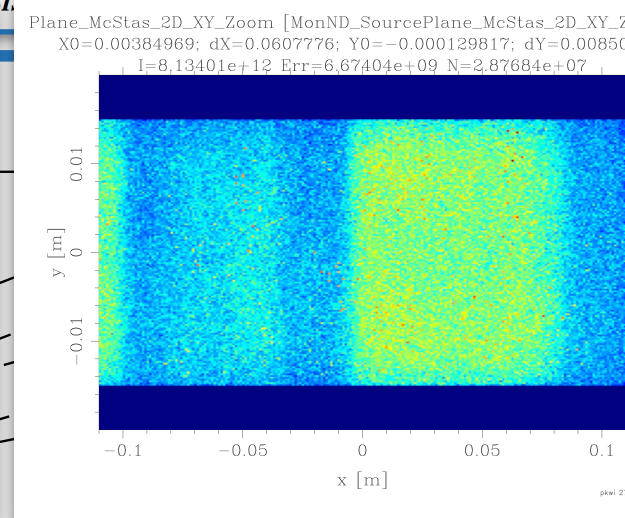
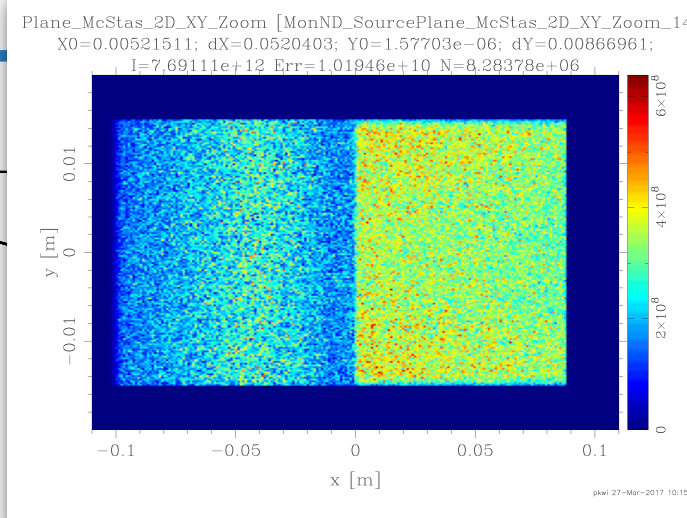
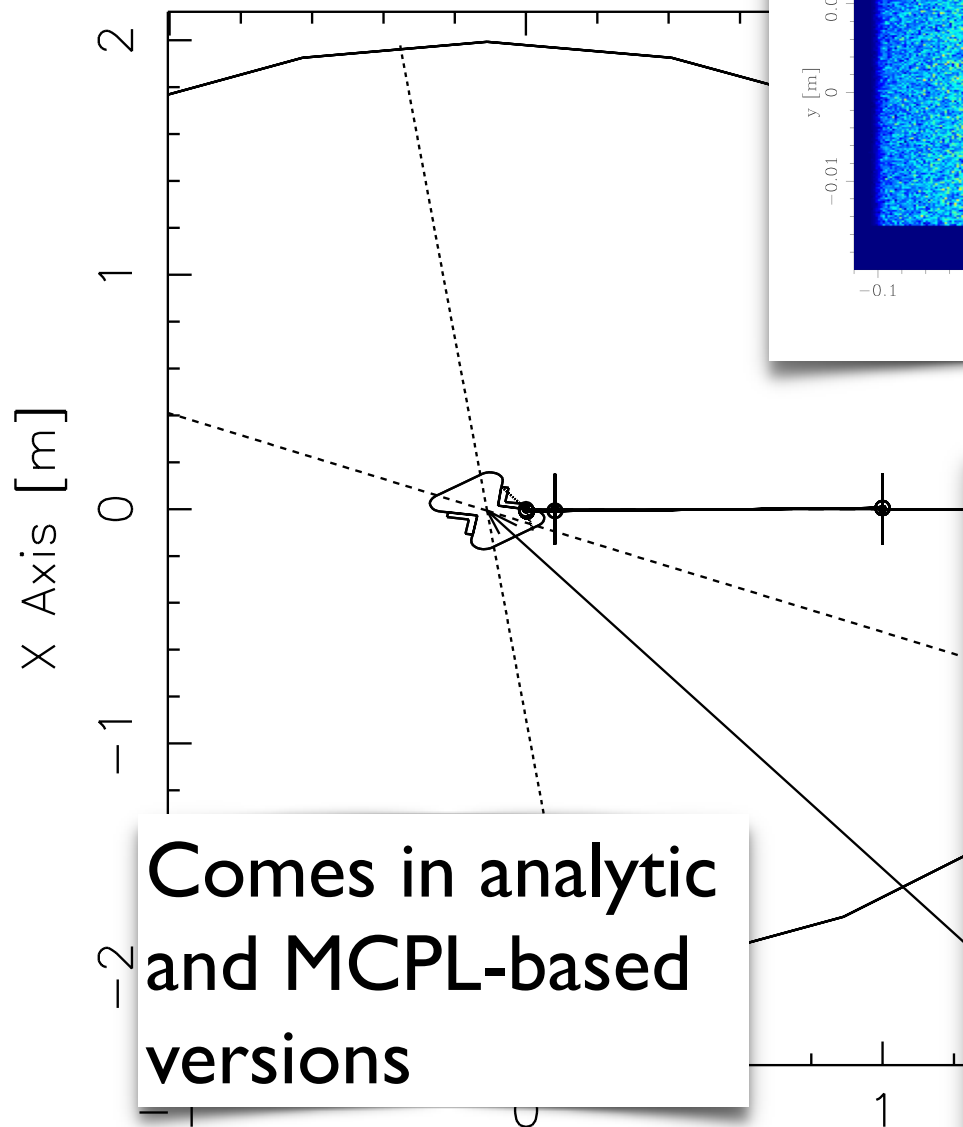
sector=N, beamline=5



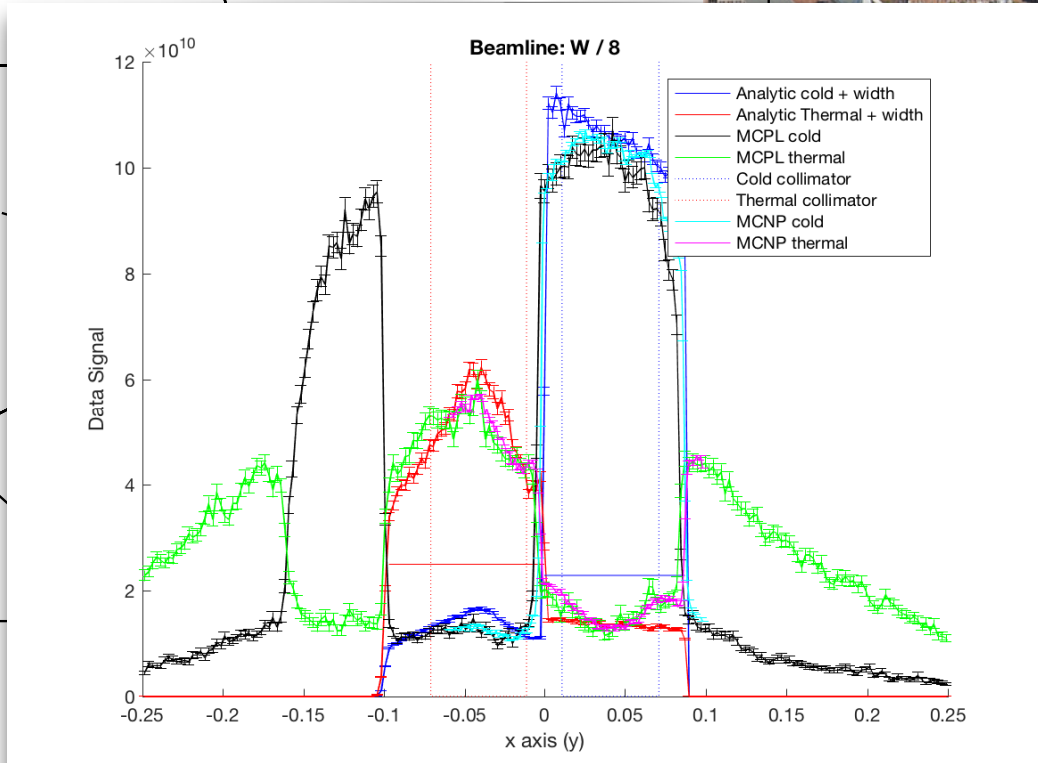
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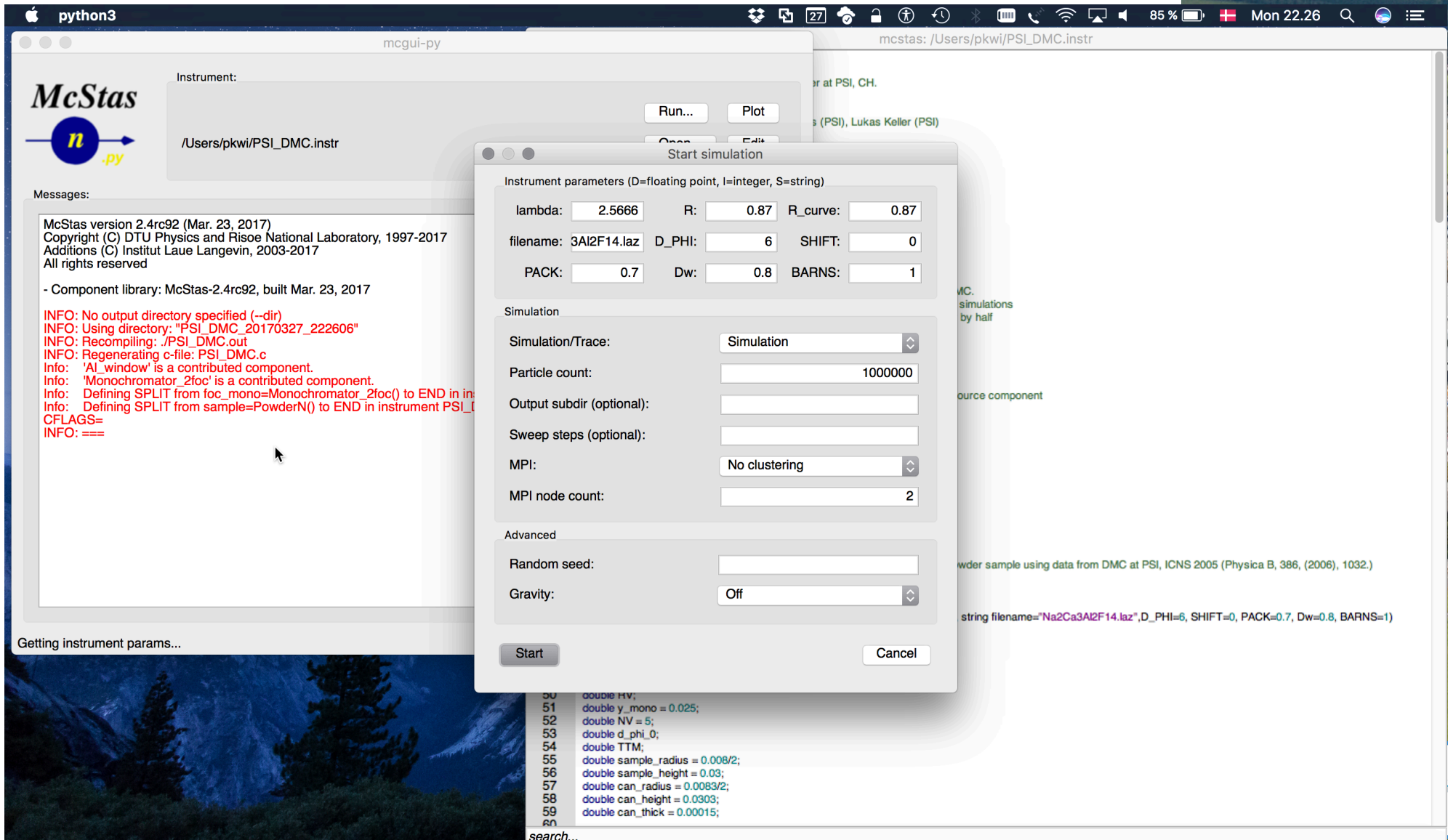


Comes in analytic and MCPL-based versions



Python tool layer default from 2.4

mcgui Tk/Perl -> PyQt + QScintilla



python3

mcgui-py

mcstas: /Users/pkwi/PSI_DMC.instr

Instrument: /Users/pkwi/PSI_DMC.instr

Run... Plot

Start simulation

Instrument parameters (D=floating point, I=integer, S=string)

lambda: 2.5666 R: 0.87 R_curve: 0.87

filename: 3AI2F14.laz D_PHI: 6 SHIFT: 0

PACK: 0.7 Dw: 0.8 BARNs: 1

Simulation

Simulation/Trace: Simulation

Particle count: 1000000

Output subdir (optional):

Sweep steps (optional):

MPI: No clustering

MPI node count: 2

Advanced

Random seed:

Gravity: Off

Start Cancel

Messages:

McStas version 2.4rc92 (Mar. 23, 2017)
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Additions (C) Institut Laue Langevin, 2003-2017
All rights reserved

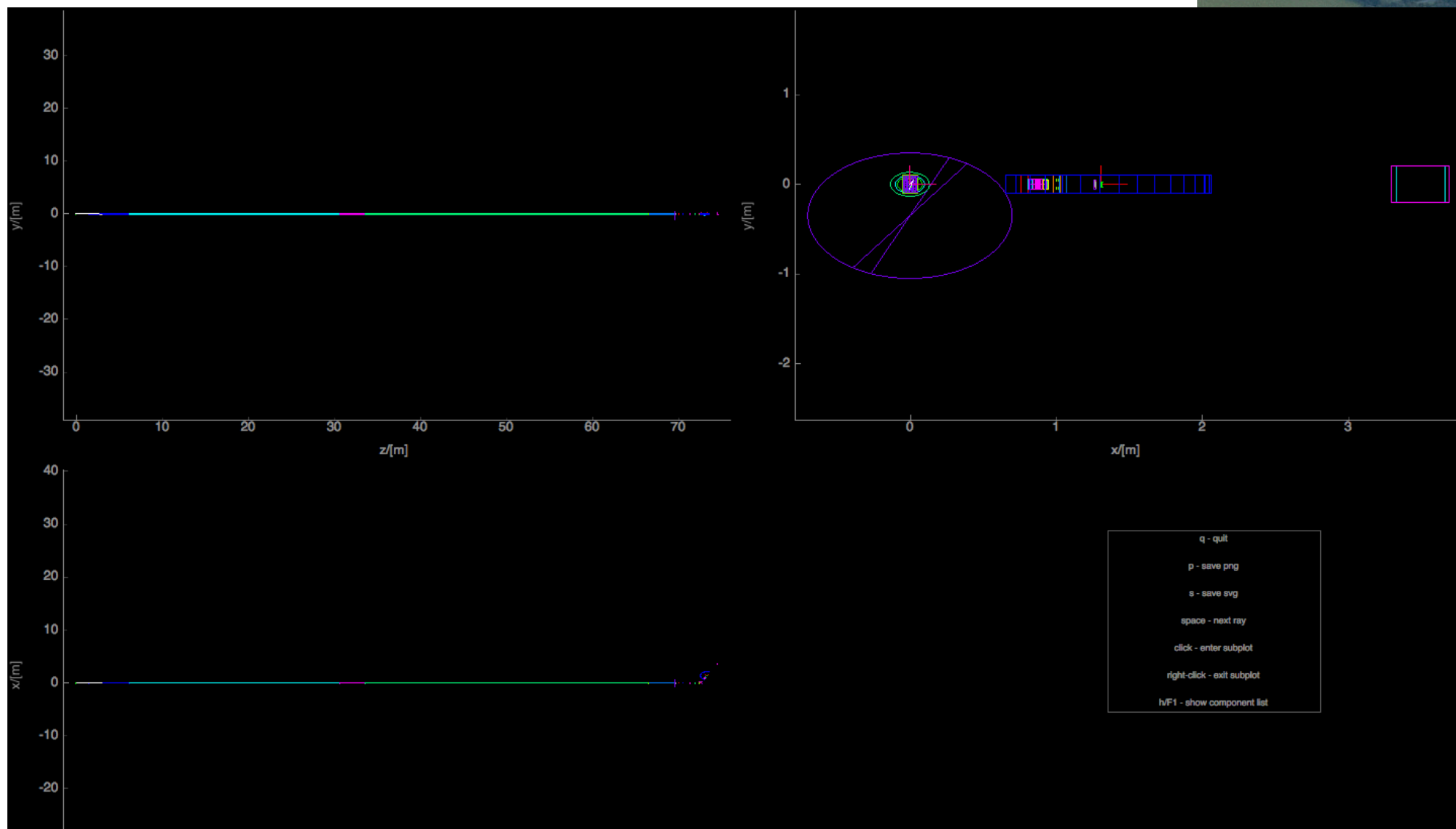
- Component library: McStas-2.4rc92, built Mar. 23, 2017

INFO: No output directory specified (--dir)
INFO: Using directory: "PSI_DMC_20170327_222606"
INFO: Recompiling: ./PSI_DMC.out
INFO: Regenerating c-file: PSI_DMC.c
Info: 'AI_window' is a contributed component.
Info: 'Monochromator_2foc' is a contributed component.
Info: Defining SPLIT from foc_mono=Monochromator_2foc() to END in in
Info: Defining SPLIT from sample=PowderN() to END in instrument PSI_
CFLAGS=
INFO: ==

```
50 double HV;  
51 double y_mono = 0.025;  
52 double NV = 5;  
53 double d_phi_0;  
54 double TTM;  
55 double sample_radius = 0.008/2;  
56 double sample_height = 0.03;  
57 double can_radius = 0.0083/2;  
58 double can_height = 0.0303;  
59 double can_thick = 0.00015;  
60
```

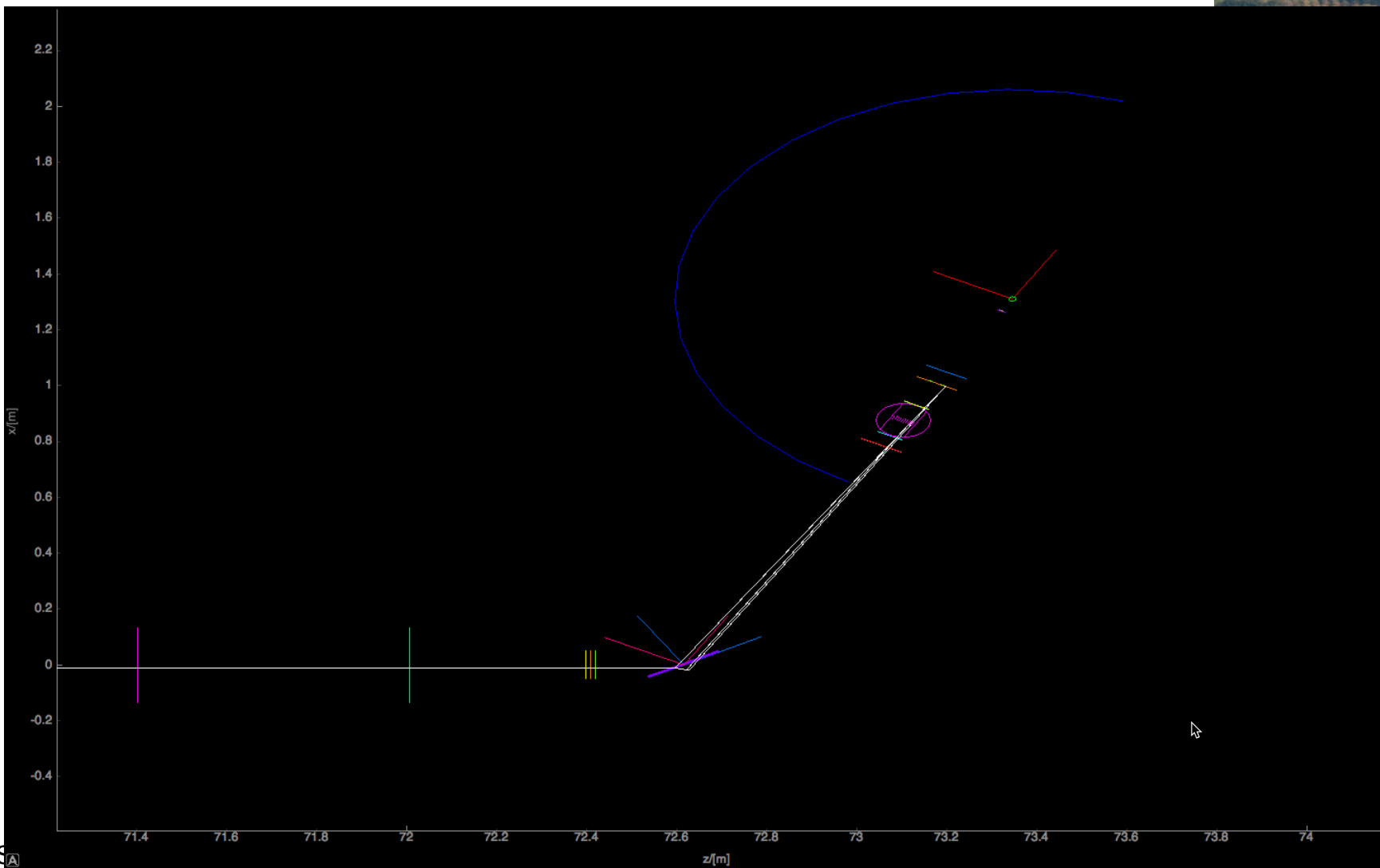
Python tool layer default from 2.4

mcdisplay Perl/PGPLOT -> PyQt + PyQtgraph



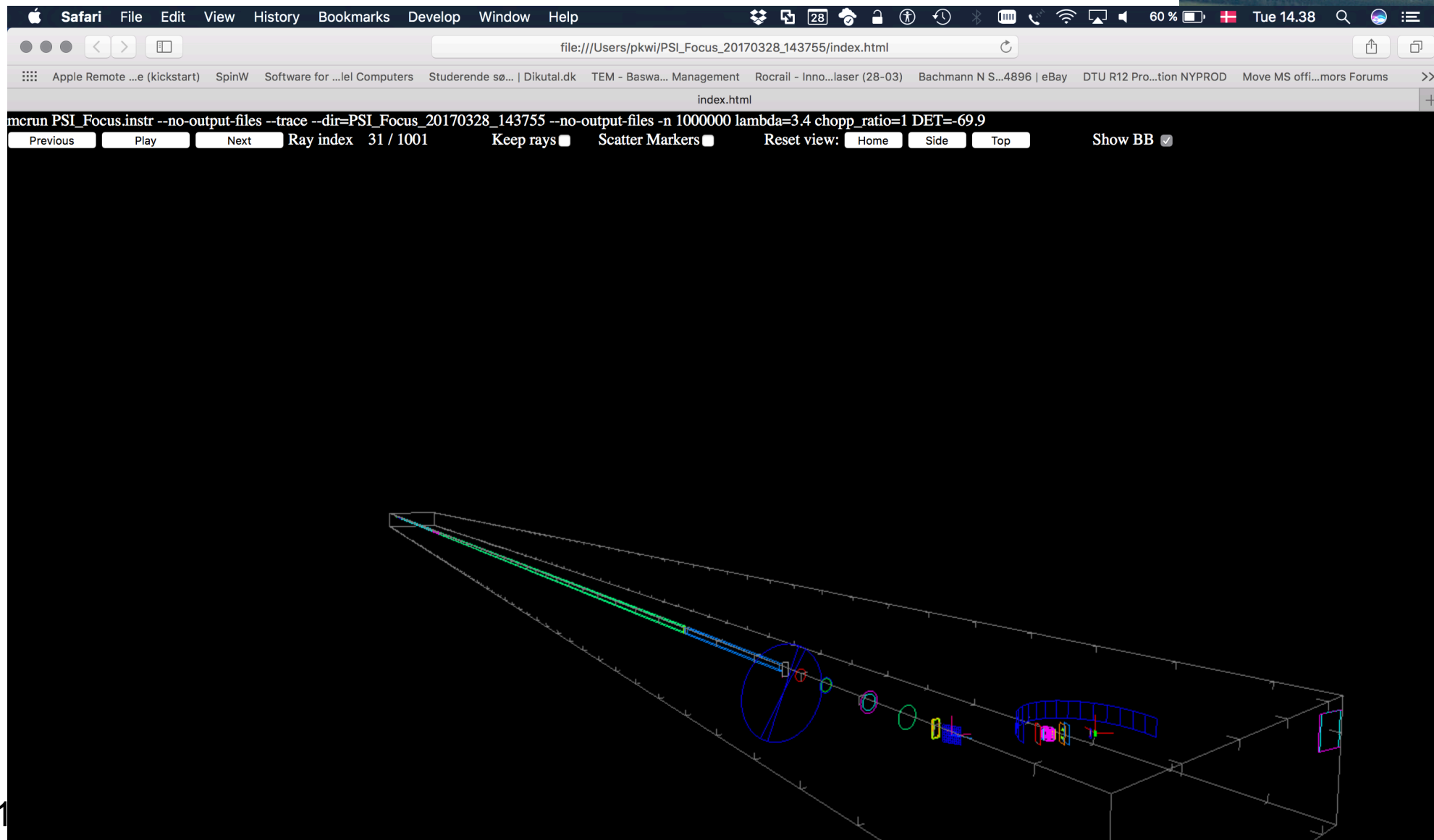
Python tool layer default from 2.4

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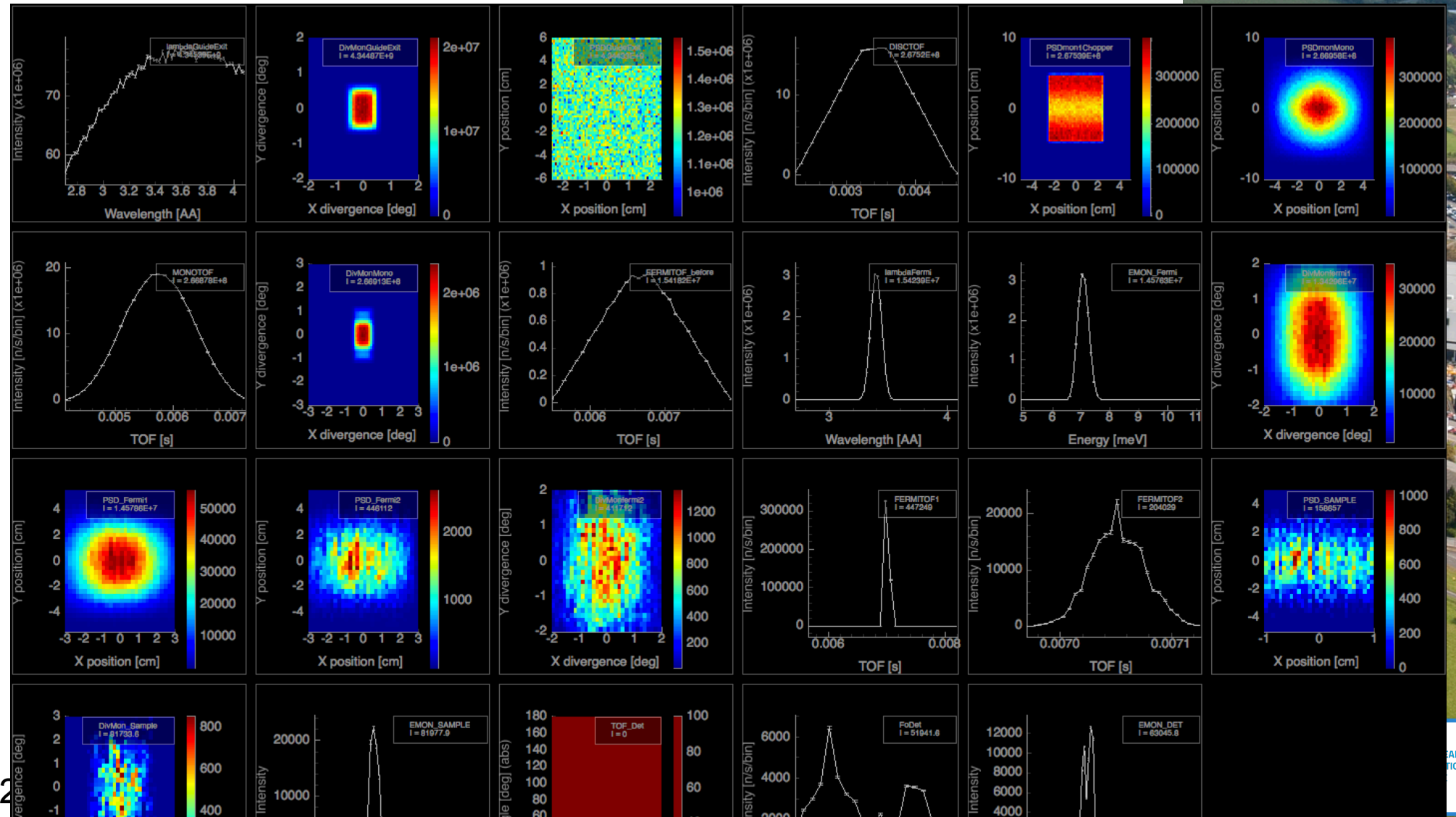
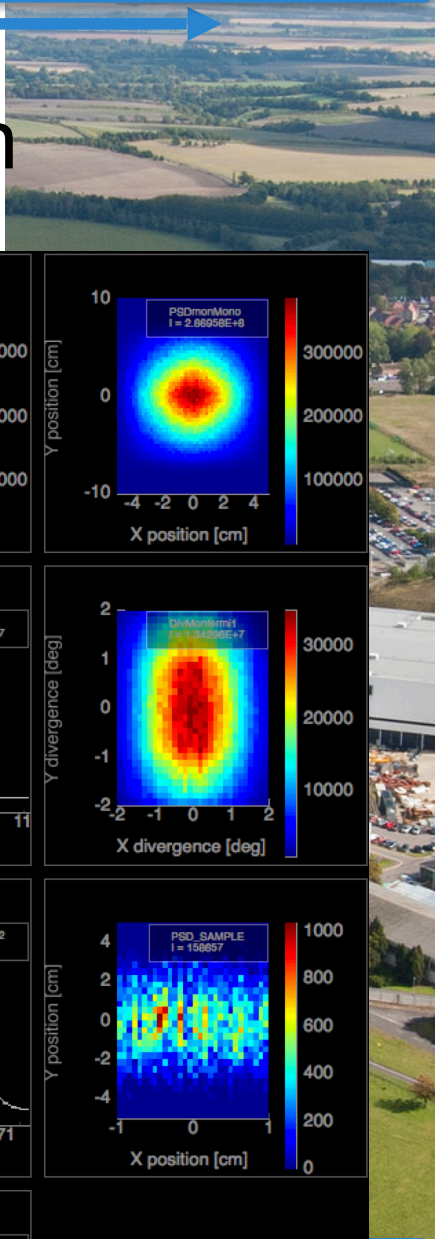
Python tool layer default from 2.4

mcdisplay Perl/PGPLOT -> Python + WebGL



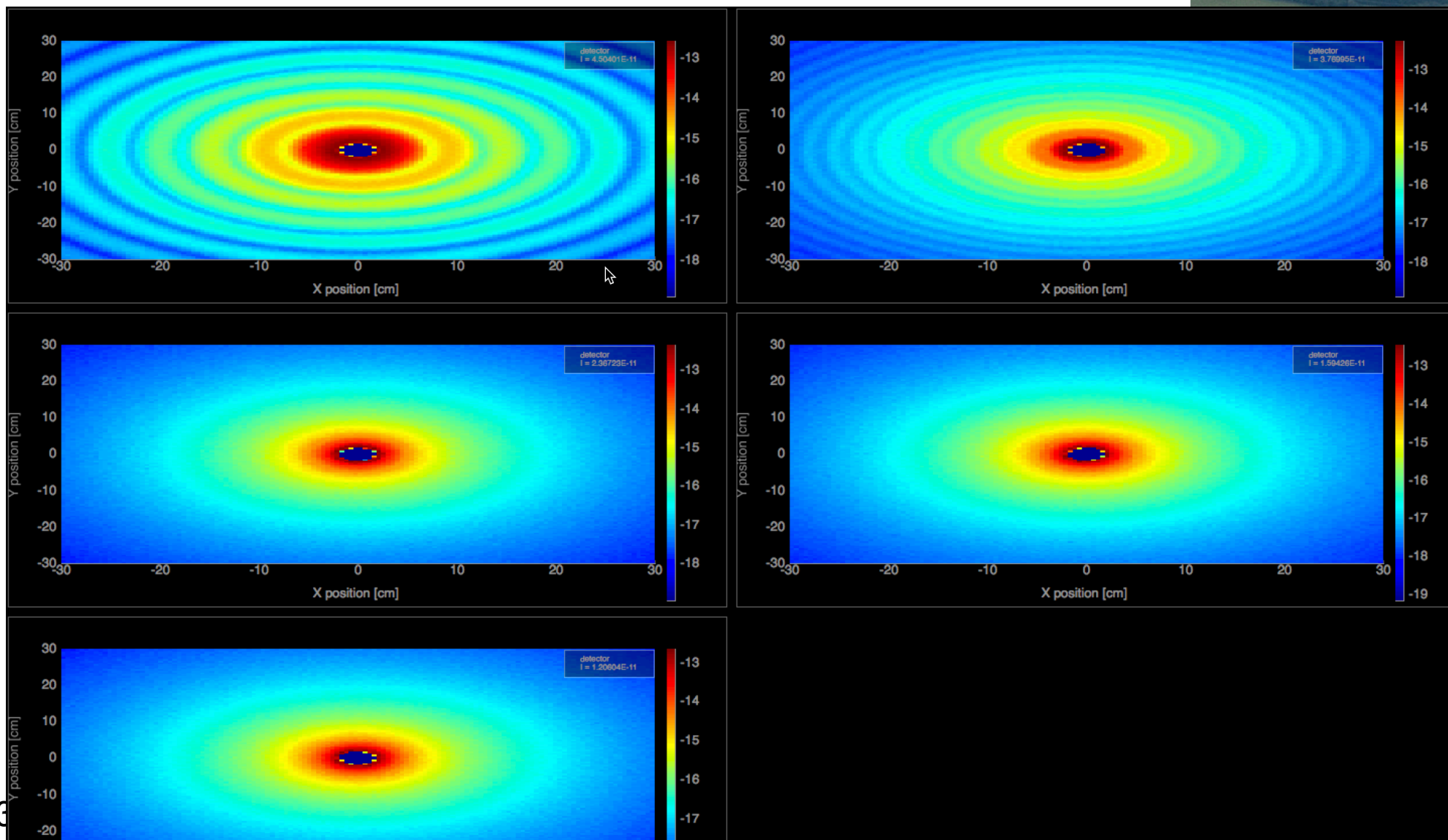
Python tool layer default from 2.4

mcplot Perl/PGPLOT -> PyQt + PyQtgraph



Python tool layer default from 2.4

mcplot Perl/PGPLOT -> PyQt + PyQtgraph

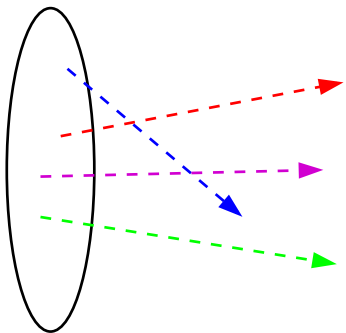




McStas overall picture

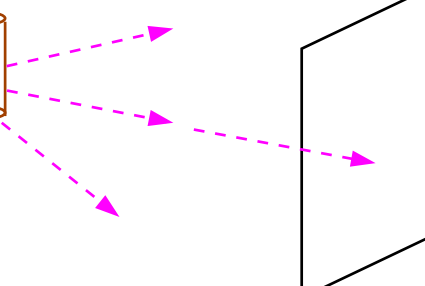
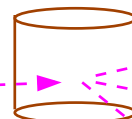
- | Important efficiency mechanisms:
 - | “Focusing” - e.g. source to beamport only (4π vs. limited solid angle only)
 - | Rather vs. single particle description, absorption handled through statistics and downscaling the ray weight

1. Particles emitted with random starting conditions via MC



2. Particles are “ray-traced” through space

3. Will eventually meet other objects e.g. a studied experimental sample and get scattered via MC again



4. At various points in the instrument the particle states are measured in so-called monitors or detectors



McStas

Algorithm limitations:

Important
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1) Linear comp seq. unless "hacks" are used

- GROUP for comps in parallel
- JUMP (a GOTO...)
- EXTEND for further free-form C-code

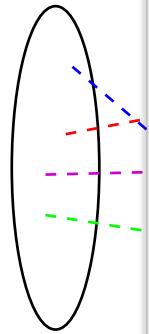
2) Multiple scattering by default "within" component only

- Some comps support "concentric" geometries e.g for sample inside sample env

3) Physics and geometry generally not separated

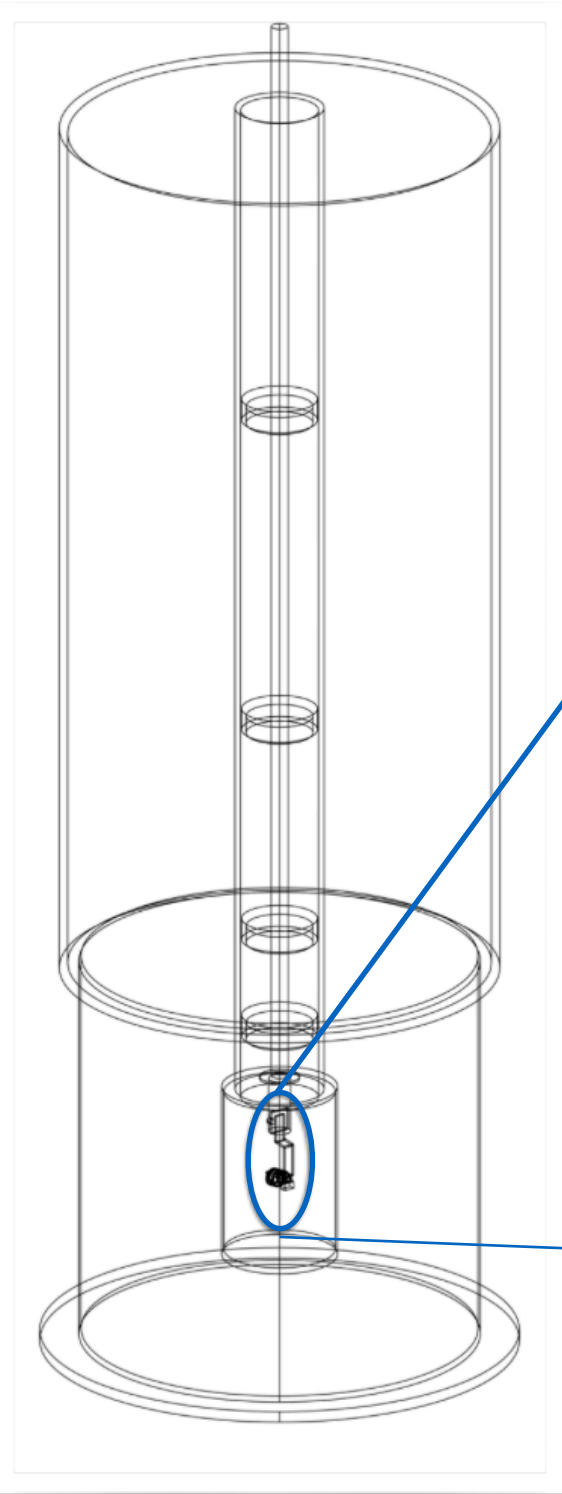
- Both a strength and weakness, simple to write new comps < 200 LoC, one place.

1. Particles emitted with random states and conditions via I



The UNION concept by **Mads Bertelsen**, KU is an attempt to do something about the above points...

points
 instrument
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 red in
 monitors
 rs



limitations:

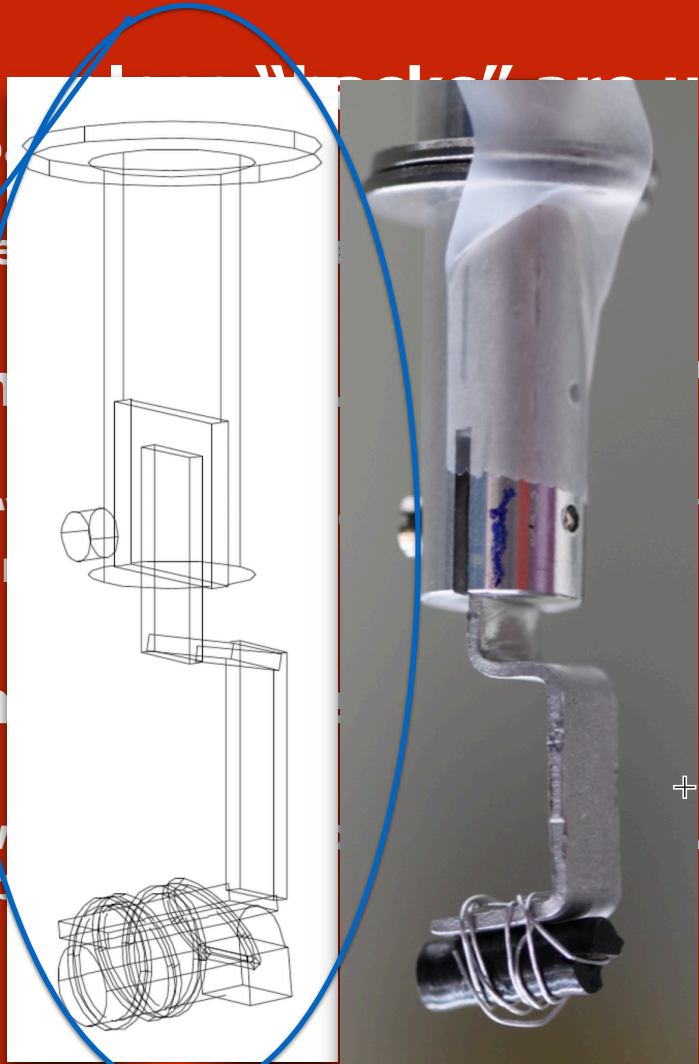
mp seq. ... "Wedge" ... sed

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LoC, one p

concept by **Mads Bertelsen**, KU is
to do something about the above



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McStas Union concept

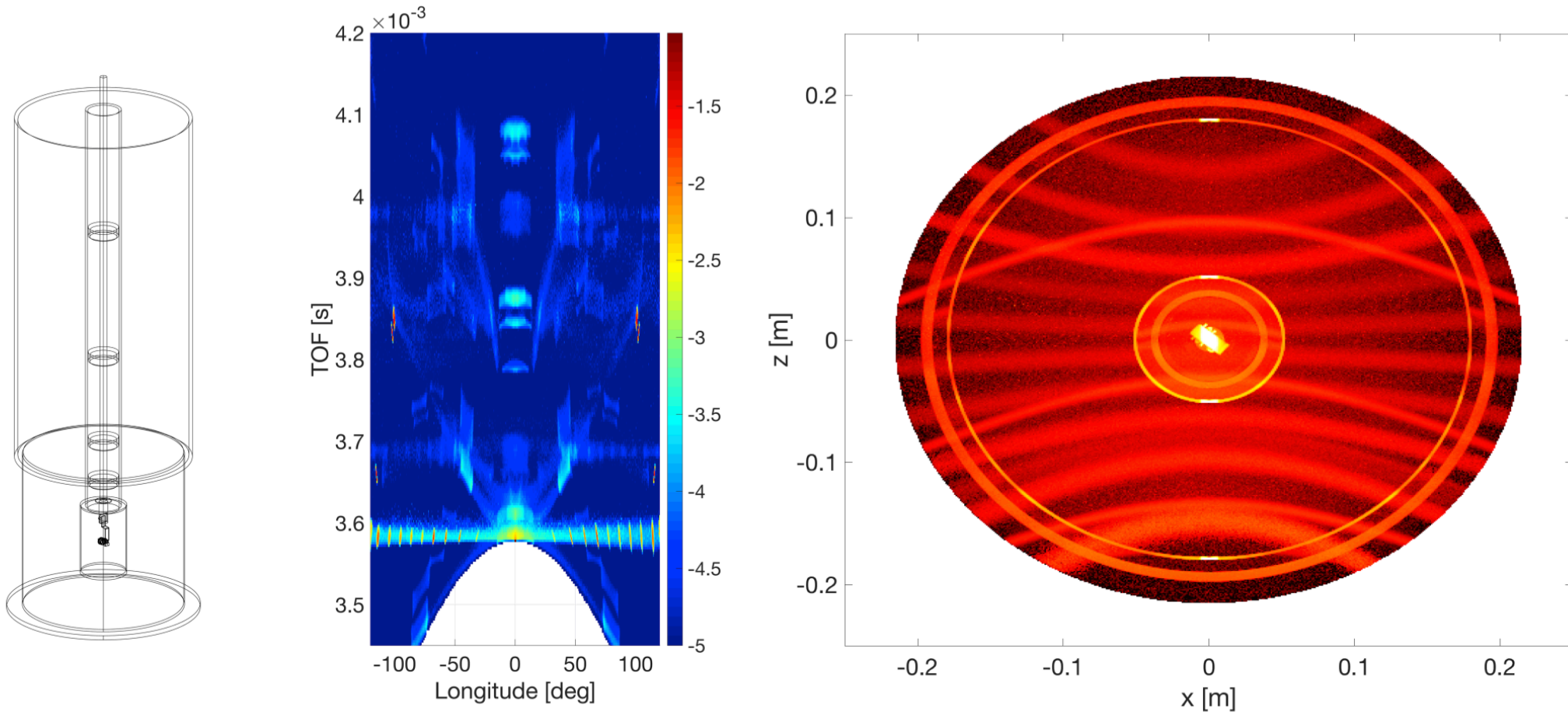


Figure 1: Left: Depiction of cryostat/sample model. Center: Time of flight banana monitor showing spurious. Right: Histogram over scattering locations in cryostat as seen from above.

See online-video at http://media.mcstas.org/ESS_DMSC_20161117/DMSC_talk_MBertelsen_McStas_Union.mp4 + ICANS XXII proceedings



Next: Demo!

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