ESS Sources in McStas - Analytic + MCPL

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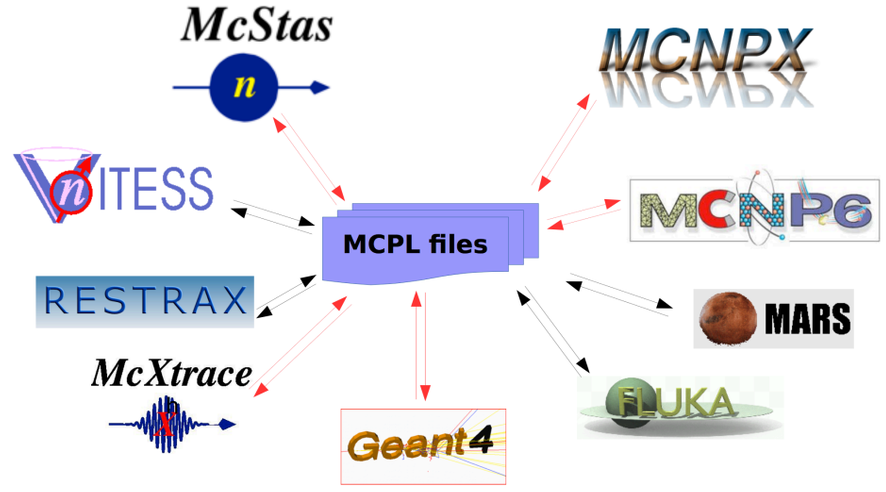
Agenda

- What is MCPL?
- “Normal” ESS source in McStas
- MCPL files and how they are generated
- Use with McStas

What is MCPL?



- MCPL is short for Monte Carlo Particle List
- Interchange-file-format for Geant4, MCNP(x), McStas etc…
- Created by T Kittelmann, ESS Detector Group, input from DTU, ESS etc.
- GitHub site: https://mctools.github.io/mcpl/
- Paper: T. Kittelmann et. al. Computer Physics Communications (218) pp. 17-42
- Talk on the subject here:
- http://coimbra2016.essworkshop.org/slides/MCPL_Kittelmann.pdf

“Normal” sources in McStas

- Describe the moderator(s) ONLY
- Describe only thermalised neutrons
- Uses analytical curves to express spectra, emission profiles etc., typically modelled using e.g. MCNP
- Advantages:
  - Fast runtime (ESS_butterfly instrument w. guide transports 1e7 neutron rays in 11 seconds on 4 cores)
  - No stat/bias issues generating further events
  - Excellent “match” for what the neutron optics can actually transport!
- Disadvantages:
  - The above issues in lacking description of high-energy particles and non-moderator particles

ESS_butterfly McDoc page:

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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 multiplicator c_performance > 0	1
t_performance	1	Thermal brilliance scalar performance multiplicator 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
tfocus_dist	m	Position of time focusing window along z axis	0
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- Choice of beamline, e.g.
  - sector=N,
  - beamline=3

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- (yheight=0.03 “fixed”)

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- cold_frac $\in$ [0,1] cold vs thermal **statistics**

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- target_index / dist "where should I aim"
- target_index = n, will point to nth component "seen from here", freeform (x,y,z)
- dist is (0,0,dist)

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- focus_xw, focus_yh
  "how much to illuminate"

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- c_ & t_performance “future penalty from engineering”

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- these you know…

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- How far to sample (flat) in time, i.e. extent of pulse + “tail”, in units of nominal pulse duration

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- How many pulses to generate, intensity remains constant (McStas sources pr. def. in units of 1/second!)

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- accelerator power (some time in the future…)

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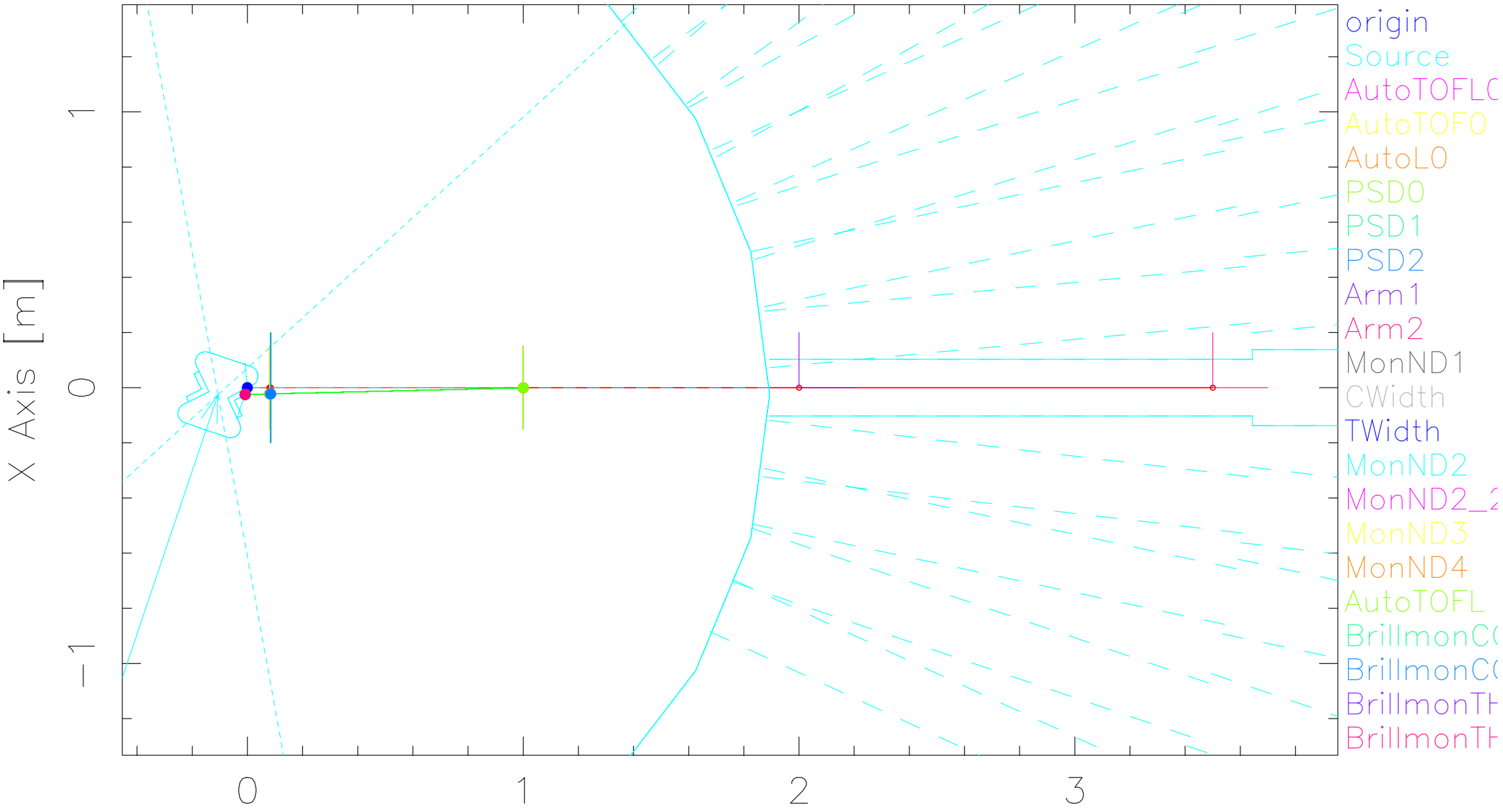
- "time-focus" at chopper window of certain duration certain distance from here

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

ESS_butterfly mcdisplay output:



http://ess_butterfly.mcstas.org/visualisation/

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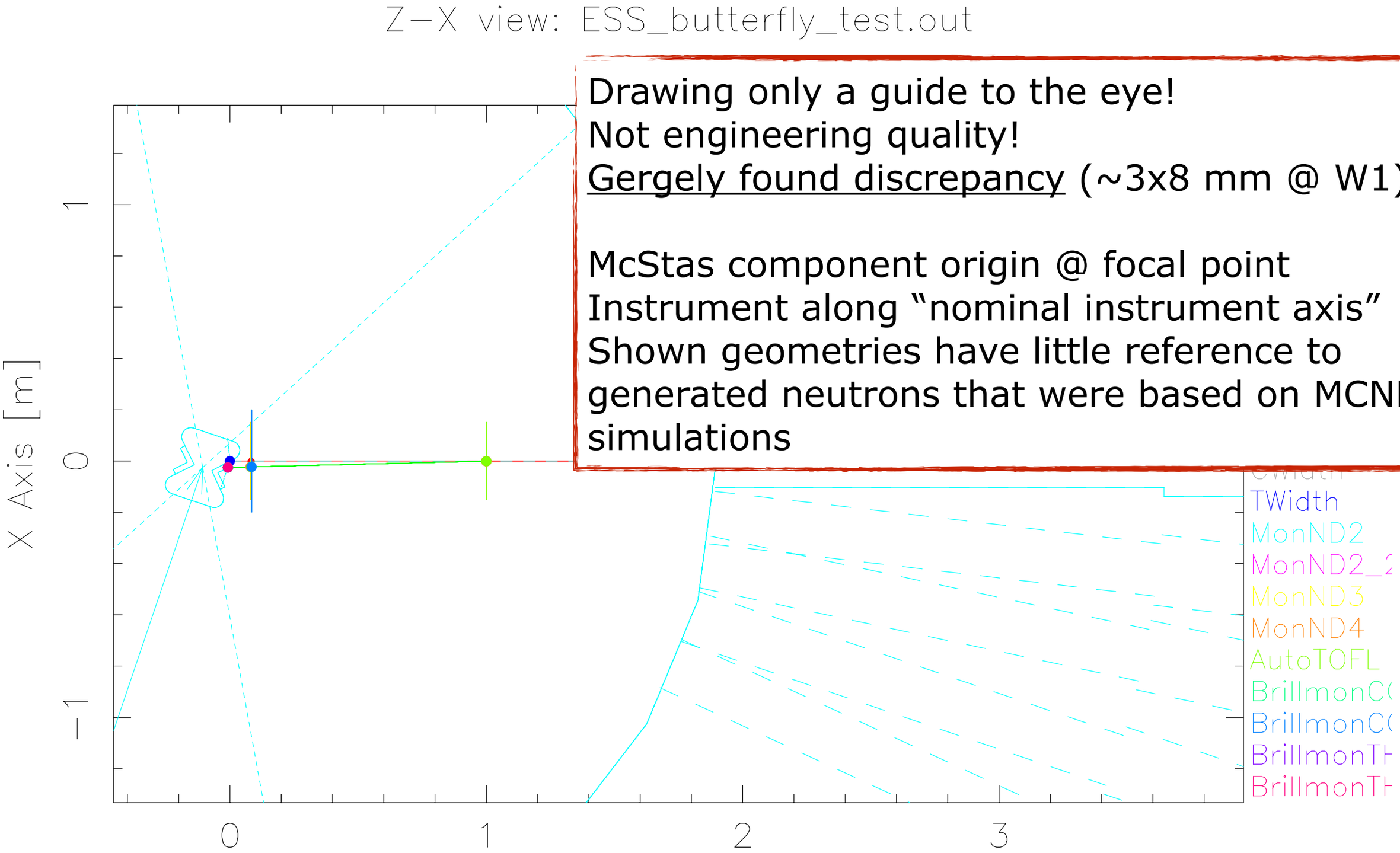


Drawing only a guide to the eye!
Not engineering quality!
Gergely found discrepancy (~3x8 mm @ W1)

McStas component origin @ focal point
Instrument along “nominal instrument axis”
Shown geometries have little reference to generated neutrons that were based on MCNP simulations

http://ess_butterfly.mcstas.org/visualisation/

MCPL files as a McStas source

- Describe any particle reaching area near the beam port, arriving from anywhere
- Describe all neutrons, any energy - but also gammas etc…
- Implemented using the SSW card in MCPN in combination with a dxtran sphere "around" beam port
- Advantages:
  - Describes anything MCNP generates, including thermalised neutrons off the reflector…
  - Could be used in attempt to model signal-to-noise @ sample, with combined McStas+MCNP transport…
- Disadvantages:
  - Stat/bias issues generating further events (simple repetition brings nothing new)
  - Files are Gb size as a starting point
  - In comparison with "normal" McStas source slow

What did Esben generate

- Dirac-delta (time) proton beam on target, 1e5 protons “NPS”.
  - I.e. McStas component/instrument includes normalisation factors
  - 1/1e5 protons/simulation -> neutrons / incoming proton
  - 1.56e16 protons/s -> neutrons / second (default McStas intensity units)
  - Uses “target” coordinate system
  - MC choice on time within pulse length

- ESS butterfly 1 design “current model”
- Simulations run for “the expected day-1 instruments”
- “dxtran sphere” used to illuminate beam port

- Size ~ 3-5Gb / beam line
- Includes ~ 1e8 particles in total
- - out of these ~50% are neutrons
- Once reduced to “transportable neutrons” ~ 1e7 events
- Takes 5-10 minutes to process through instr w/guide if not filtered in any way…

MCPL_input component interface

Description

```
Source-like component that reads neutron state parameters from a binary mcpl-file.

MCPL is short for Monte Carlo Particle List, and is a new format for sharing events
between e.g. MCNP(X), Geant4 and McStas.

When used with MPI, the --ncount given on the commandline is overwritten by
#MPI nodes x #events in the file.

%BUGS
```

Generic, no reference to “ess” in this

Input parameters

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

- https://mctools.github.io/mcpl/

Name	Unit	Description	Default
filename	str	Name of neutron mcpl file to read.	0
polarisationuse		If !=0 read polarisation vectors from file.	1
verbose		Print debugging information for first 10 particles read.	1
Emin	meV	Lower energy bound. Particles found in the MCPL-file below the limit are skipped.	0
Emax	meV	Upper energy bound. Particles found in the MCPL-file above the limit are skipped.	FLT_MAX
repeat_count	1	Repeat contents of the MCPL file this number of times. NB: When running MPI, repeating is implicit and is taken into account by integer division. Should be combined sith the _smear options!	1
E_smear	1	When repeating events, make a Gaussian MC choice within E_smear*E around particle energy E	0
pos_smear	m	When repeating events, make a flat MC choice of position within pos_smear around particle starting position	0
dir_smear	deg	When repeating events, make a Gaussian MC choice of direction within dir_smear around particle direction	0

- See also:
  - https://arxiv.org/abs/1609.02792
  - https://mctools.github.io/mcpl/
  - http://coimbra2016.essworkshop.org/slides/MCPL_Kittelmann.pdf

ESS sources in McStas

MCPL_output component interface

Description

```
Detector-like component that writes neutron state parameters into an mcpl-format
binary, virtual-source neutron file.

MCPL is short for Monte Carlo Particle List, and is a new format for sharing events
between e.g. MCNP(X), Geant4 and McStas.

When used with MPI, the component will output #MPI nodes individual MCPL files that
can be merged using the mcpltool.

MCPL_output allows a few flags to tweak the output files:
1. If use_polarisation is unset (default) the polarisation vector will not be stored (saving space)
2. If doubleprec is unset (default) data will be stored as 32 bit floating points, effectively cutting the output file size in half.
3. Extra information may be attached to each ray in the form of a userflag, a user-defined variable wich is packed into 32 bits. If
the user variable does not fit in 32 bits the value will be truncated and likely garbage. If more than one variable is to be attached to
each neutron this must be packed into the 32 bits.

These features are set this way to keep file sizes as manageable as possible.

%BUGS
```

Input parameters

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

Name	Unit	Description	Default
polarisationuse	1	Enable storing the polarisation state of the neutron.	0
doubleprec	1	Use double precision storage	0
verbose	1	If 1) Print summary information for created MCPL file. 2) Also print summary of first 10 particles information stored in the MCPL file. >2) Also print information for first 10 particles as they are being stored by McStas.	0
userflag	1	Extra variable to attach to each neutron. The value of this variable will be packed into a 32 bit integer.	0
filename	str	Name of neutron file to write. Default is standard output [string]. If not given, a unique name will be used.	0
userflagcomment	str	String variable to describe the userflag. If this string is empty (the default) no userflags will be stored.	""
merge_mpi	1	Flag to indicate if output should be merged in case of MPI	1
keep_mpi_unmerged	1	Flag to indicate if original unmerged mcpl-files should be kept (or deleted).	0

- See also:
  - https://arxiv.org/abs/1609.02792
  - https://mctools.github.io/mcpl/
  - http://coimbra2016.essworkshop.org/slides/MCPL_Kittelmann.pdf

Inserted in instrument file for ESS context

ESS_butterfly_MCPL_test.html

```
COMPONENT Origin = Progress_bar()
AT (0, 0, 0) ABSOLUTE

/* read neutrons from an mcpl file*/

COMPONENT vinROT2 = Arm()
AT(0,0,0) RELATIVE PREVIOUS
  ROTATED (0,-90,0) RELATIVE PREVIOUS

COMPONENT vinROT1 = Arm()
AT(0,0,0) RELATIVE PREVIOUS
  ROTATED (-90,0,0) RELATIVE PREVIOUS

COMPONENT vin = MCPL_input(filename=MCPLfile,verbose=1,repeat_count=repeat,E_smear=E_smear,pos_smear=pos_smear,dir_smear=dir_smear)
AT(0,0,0) RELATIVE PREVIOUS
EXTEND %{
  if(p>mcipthres) {ABSORB;}
  else {SCATTER;}
  p*=1.56e16;
  p/=1e5;
  z=z-0.137;
%}

COMPONENT Sphere1 = PSD_monitor_4PI(filename="nonrotated", radius=2.2,restore_neutron=1)
AT (0,0,0) RELATIVE PREVIOUS

/* Focusing for this use of the source is a little unphysical: 1x1cm @ 1m ~ 1e-4 steradian. To be useful in a "proper" instrument, you should of course illuminate your beamport
lly!*/
COMPONENT Source = ESS_butterfly(sector=sector,beamline=beamline,Lmin=Lmin,Lmax=Lmax,c_performance=c_performance,t_performance=t_performance,dist=dist,target_index=index,cold_f
=cold, yheight=Yheight,
                                 focus_xw=0.01, focus_yh=0.01)
  WHEN (0==1) AT (DeltaX,0,DeltaZ) ABSOLUTE
  ROTATED (0, ANGLE, 0) ABSOLUTE
```

Default parameters for “repeating events”

- All mpi nodes read the file fully and independently… So we’d better do something clever….

- E_smear=0.1 ~ MC choice of energy in Gaussian of sigma 0.1*E_0
- pos_smear=0.01 ~ MC choice on position within sphere of radius 0.01m
- dir_smear=0.01 ~ MC choice on direction within cone of 0.01 deg

- repeat=N gives a repetition of the events in the file by ceil(N/mpicount)
  - (10 reps over 4 nodes ~ 3 reps pr node ~ 12 reps)

- MC choice applied for nodes of rank > 1 and when file is being repeated at individual node.

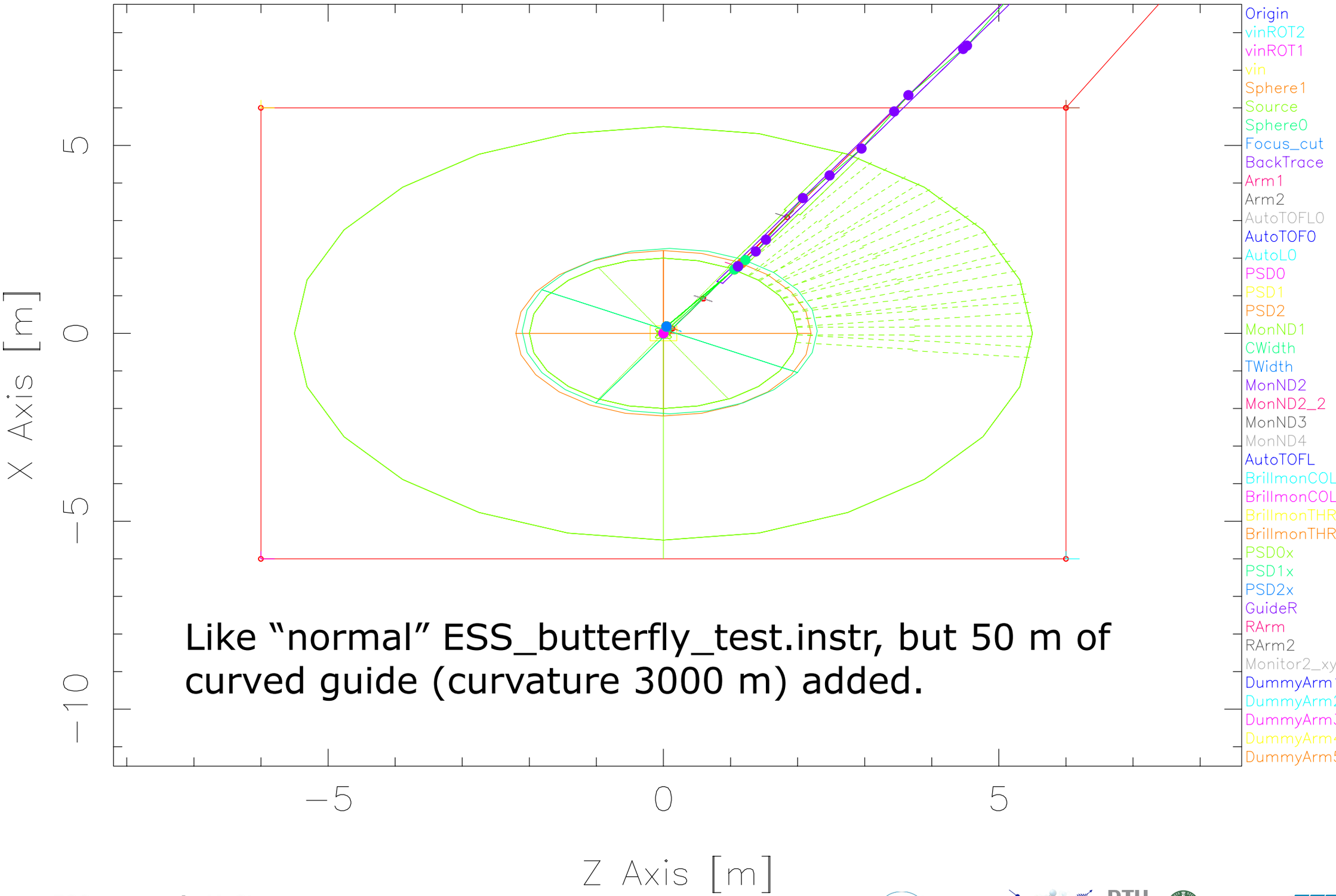
!! Caution !!

Smear-settings are user parameters - but can clearly be misused! Make conservative choices here, base on physical / geometrical considerations please!

- E_smear=0.1 ~ MC choice of energy in Gaussian of sigma 0.1*E_0
- pos_smear=0.01 ~ MC choice on position within sphere of radius 0.01m
- dir_smear=0.01 ~ MC choice on direction within cone of 0.01 deg

- repeat=N gives a repetition of the events in the file by ceil(N/mpicount)
  - (10 reps over 4 nodes ~ 3 reps pr node ~ 12 reps)

- MC choice applied for nodes of rank > 1 and when file is being repeated at individual node.



Like “normal” ESS_butterfly_test.instr, but 50 m of curved guide (curvature 3000 m) added.

For the McStas users…

- Template instrument file creates similar interface as for the “analytical” ESS_butterfly, pick your sector and beam line and you are good to go!

- sector=W beamline=8 -> reads W8.mcpl.gz (with filter=1 reads W8_filtered.mcpl.gz)

- Plan on expanding this kind of logic and provide a set of “onion-shelled” MCPL files pr. beam line (filters on particle type, energy, position, divergence etc…)

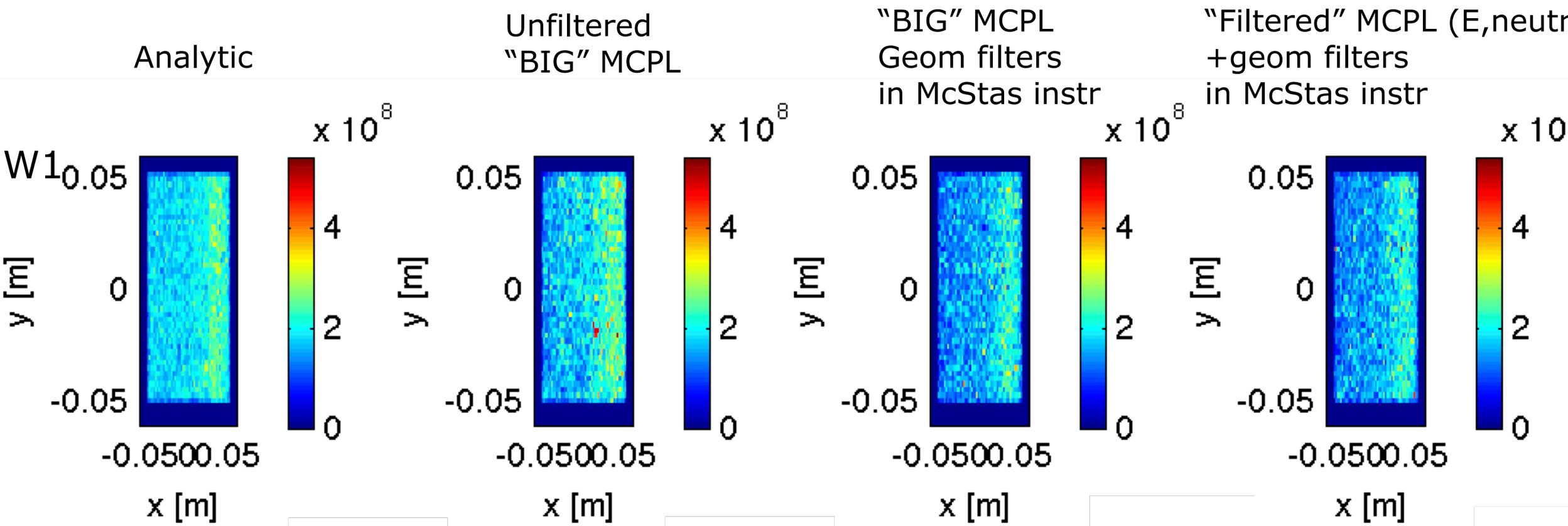
- Full documentation with examples will become available on Atlassian

- Files will be served on the DMSC cluster

Analytic vs. event models - PSD after curved guide

	Intensity	# events
Analytic:	3.58867e+11	9.88961e+06
Unfiltered BIG:	3.54106e+11	7.55581e+07
McStas filtered BIG:	3.01198e+11	1.49028e+07
Filtered MCPL:	3.01273e+11	1.48899e+07

Good agreement,
1) Pics below similar
2) ~ Same intensity



50 sec **5.5 min** **2.6 min** **1.3 min**

Execution times…

Which source to use when??

- **Frontend** optimisation, final “placement”:
  I would probably use MCPL based source, but with caution

- Anything beyond that / requiring “proper stats”:
  Use analytic source

Web resources…

- Confluence page "Using MCPL as source term in McStas"
- ESS_butterfly "benchmarking website" w/reports etc.
- MCPL input files describing ESS beamlines