

# ESS Sources in McStas - Analytic + MCPL

Peter Willendrup<sup>1,3</sup>, Esben Klinkby<sup>2,4</sup>

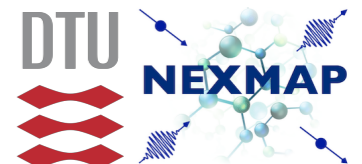
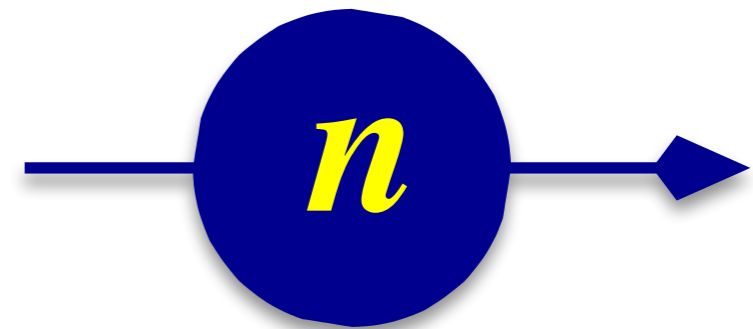
<sup>1</sup>Physics Department, Technical University of Denmark, Denmark

<sup>2</sup>Center for Nuclear Technologies, Technical University of Denmark

<sup>3</sup>ESS DMSC, Copenhagen, Denmark

<sup>3</sup>ESS, Lund, Sweden

# *McStas*

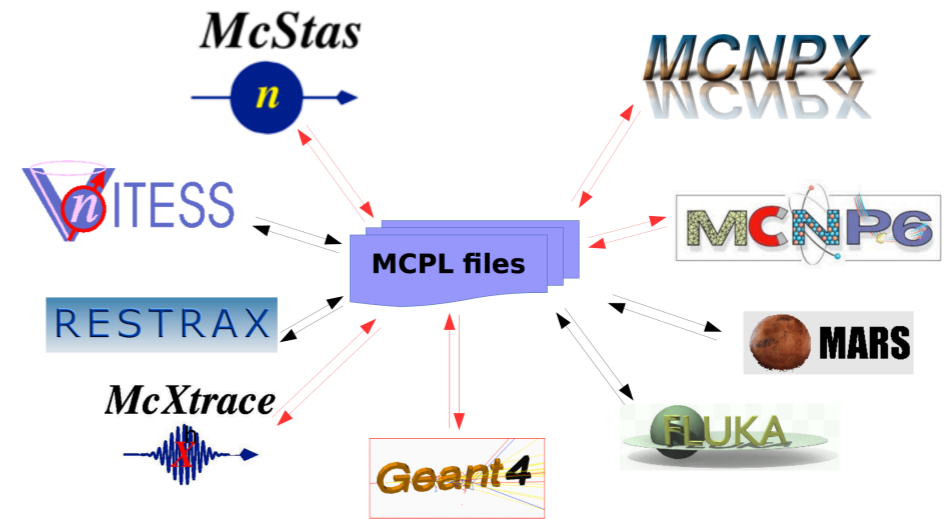


# Agenda

- 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](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:

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/](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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas



# 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/](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	su	Defines the 'sector' of your instrument position. Val	"N"
beamline	1	Defines the 'beamline number' of your instrument p	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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

- Choice of beamline, e.g.
  - sector=N,
  - beamline=3

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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 11 depending on sector	1
yheight	m	Defines the moderator height. Valid values are 0.03	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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• (yheight=0.03 "fixed")

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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	0.03
<b>cold_frac</b>	1	Defines the statistical fraction of events emitted from cold moderator	0.5
target_index	1	Relative index of component to focus at, e.g. next is	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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• cold\_frac  $\in [0,1]$  cold vs thermal **statistics**

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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 cold moderator	0.5
target_index	1	Relative index of component to focus at, e.g. next is 1, then 2, then 3	0
dist	m	Distance from origin to focusing rectangle; at (0,0,dist)	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_perform	1
t_performance	1	Thermal brilliance scalar performance multiplier t_perform	1
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

- 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)

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas



# 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/](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) <del>alternative name: target_index</del>	0
focus_xw	m	<del>Width of focusing rectangle</del>	0
focus_yh	m	<del>Height of focusing rectangle</del>	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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• focus\_xw, focus\_yh  
"how much to illuminate"

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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
<del>c_performance</del>	<del>1</del>	<del>Cold brilliance scalar performance multiplier</del>	<del>1</del>
<del>t_performance</del>	<del>1</del>	<del>Thermal brilliance scalar performance multiplier</del>	<del>1</del>
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• c\_ & t\_performance "future penalty from engineering"

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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 multiplicator $c\_performance > 0$	1
t_performance	1	Thermal brilliance scalar performance multiplicator $t\_performance > 0$	1
<b>Lmin</b>	<b>AA</b>	<del>Minimum wavelength simulated</del>	
<b>Lmax</b>	<b>AA</b>	<del>Maximum wavelength simulated</del>	
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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• these you know...

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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 multiplicator $c\_performance > 0$	1
t_performance	1	Thermal brilliance scalar performance multiplicator	1
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	AA	Maximum wavelength simulated	
tmax_multiplic	1	Defined maximum emission time at moderator, tmax	3
n_pulses	1	Number of pulses simulated. 0 and 1 creates one pul	1
acc_power	MW	Accelerator power in MW	5
tfocus_dist	m	Position of time focusing window along z axis	0
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

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

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	AA	Maximum wavelength simulated	
tmax_multiplier	1	Defined maximum emission time at moderator, tmax	3
<b>n_pulses</b>	1	Number of pulses simulated. 0 and 1 creates one pul	1
acc_power	MW	Accelerator power in MW	5
tfocus_dist	m	Position of time focusing window along z axis	0
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

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

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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 pul	1
acc_power	MW	Accelerator power in MW	5
tfocus_dist	m	Position of time focusing window along z axis	0
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

• accelerator power (some time in the future...)

- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas

# 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/](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 multiplicator $c\_performance > 0$	1
t_performance	1	Thermal brilliance scalar performance multiplicator $t\_performance > 0$	1
<b>Lmin</b>	AA	Minimum wavelength simulated	
<b>Lmax</b>	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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

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

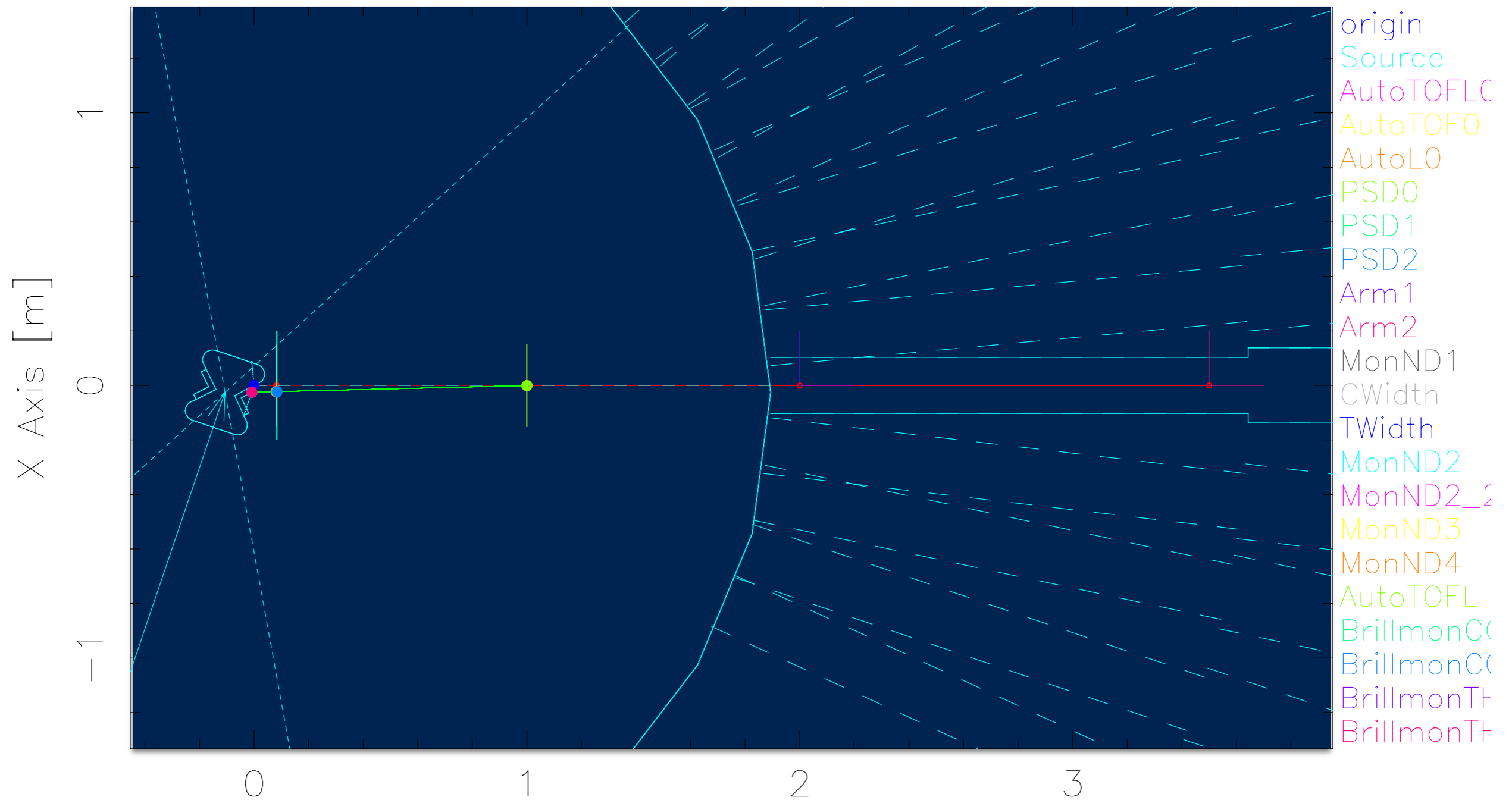
- See also [http://ess\\_butterfly.mcstas.org](http://ess_butterfly.mcstas.org)

ESS sources in McStas



# ESS\_butterfly mcdisplay output:

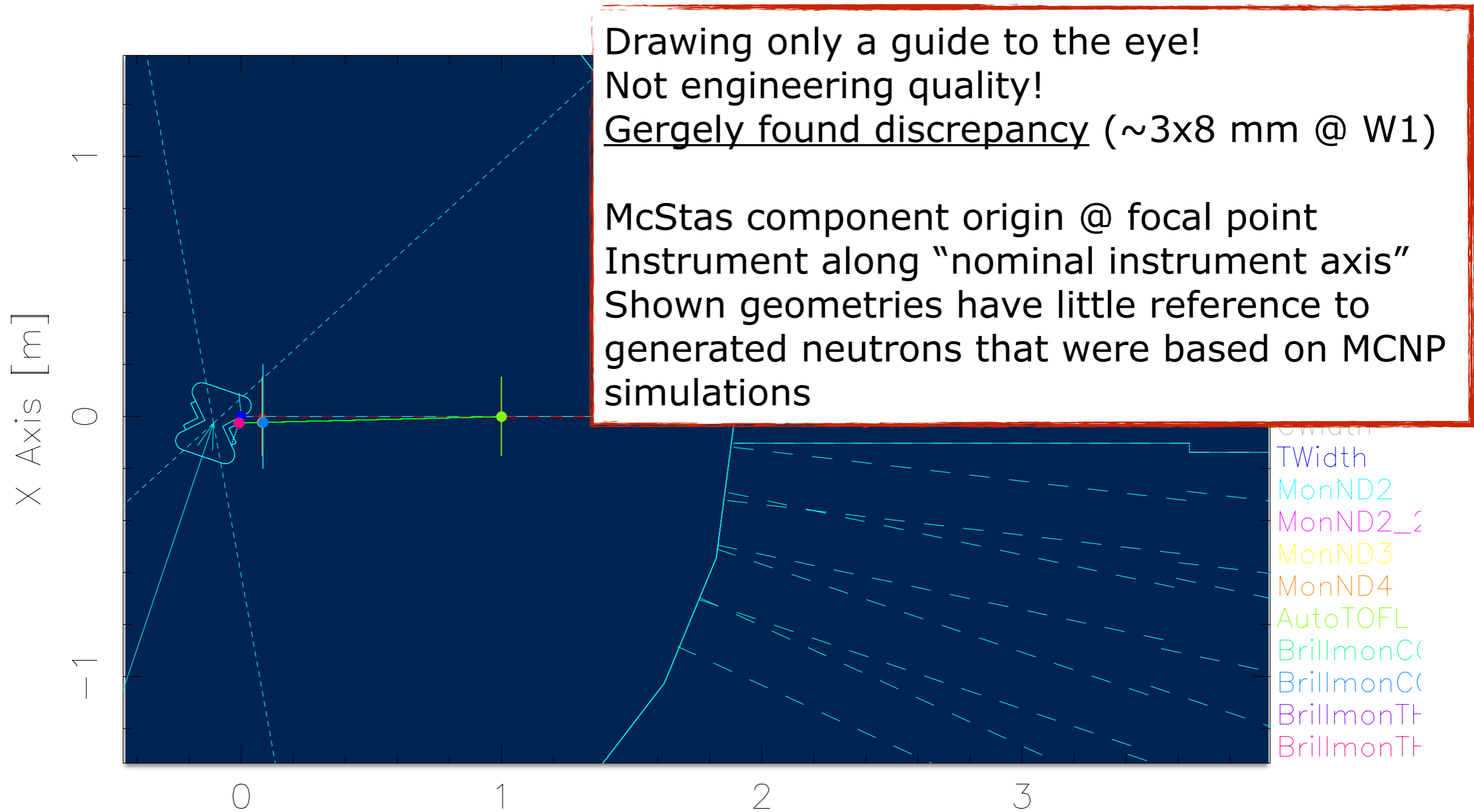
Z-X view: ESS\_butterfly\_test.out



[http://ess\\_butterfly.mcstas.org/visualisation/](http://ess_butterfly.mcstas.org/visualisation/)

# ESS\_butterfly mcdisplay output:

Z-X view: ESS\_butterfly\_test.out



[http://ess\\_butterfly.mcstas.org/visualisation/](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  $\rightarrow$  neutrons / incoming proton
  - $1.56e16$  protons/s  $\rightarrow$  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  $\sim 3-5$ Gb / beam line
- Includes  $\sim 1e8$  particles in total
- - out of these  $\sim 50\%$  are neutrons
- Once reduced to "transportable neutrons"  $\sim 1e7$  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 with 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](http://coimbra2016.essworkshop.org/slides/MCPL_Kittelmann.pdf)

ESS sources in McStas



# Description **MCPL\_output component interface**

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 which 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](http://coimbra2016.essworkshop.org/slides/MCPL_Kittelmann.pdf)

ESS sources in McStas

# 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>mciphres) {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 fully!*/
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”

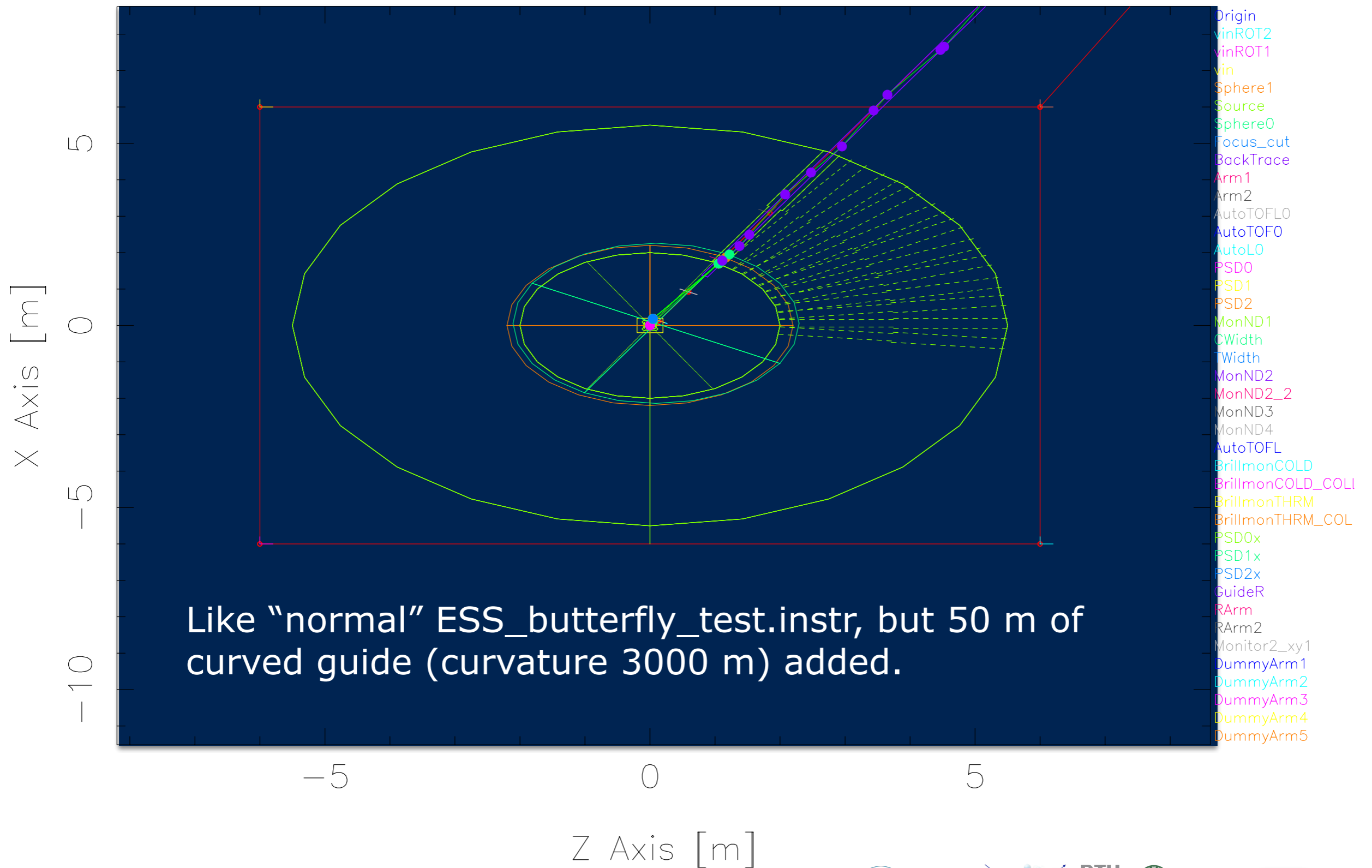
- All mpi nodes read the file fully and independently... So we'd better do something clever....
- $E\_smear=0.1$  ~ MC choice of energy in Gaussian of sigma  $0.1 * E_0$
- $pos\_smear=0.01$  ~ MC choice on position within sphere of radius 0.01m
- $dir\_smear=0.01$  ~ MC choice on direction within cone of 0.01 deg
- $repeat=N$  gives a repetition of the events in the file by  $\text{ceil}(N/\text{mpicount})$ 
  - (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!**

- $E_{\text{smear}}=0.1$  ~ MC choice of energy in Gaussian of sigma  $0.1 \cdot E_0$
- $\text{pos\_smear}=0.01$  ~ MC choice on position within sphere of radius 0.01m
- $\text{dir\_smear}=0.01$  ~ MC choice on direction within cone of 0.01 deg
  
- $\text{repeat}=N$  gives a repetition of the events in the file by  $\text{ceil}(N/\text{mpicount})$ 
  - (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.

Z-X view: ESS\_butterfly\_MCPL\_NOFILTERtest.out



# 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

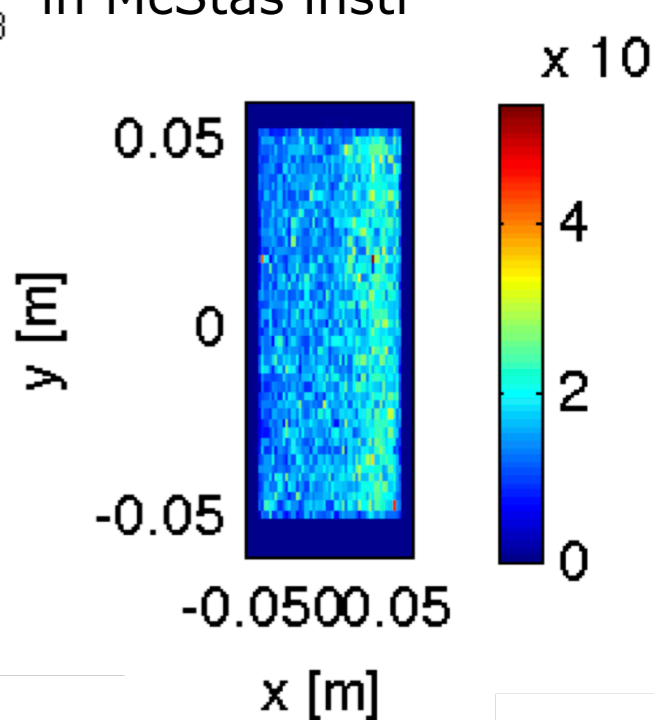
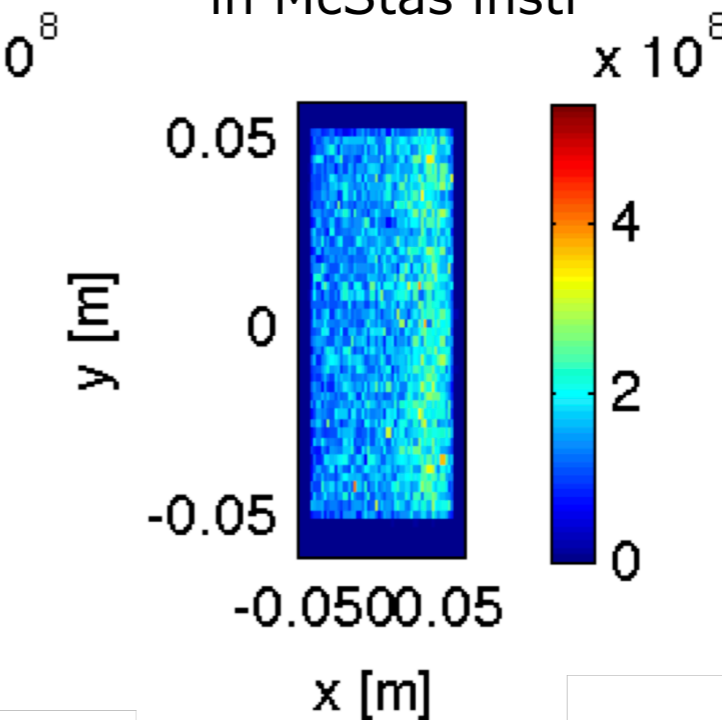
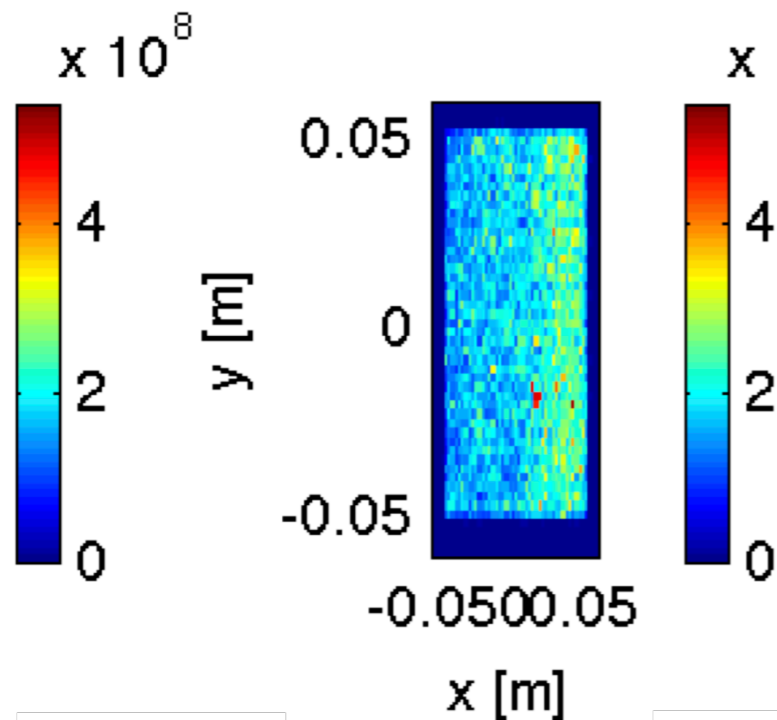
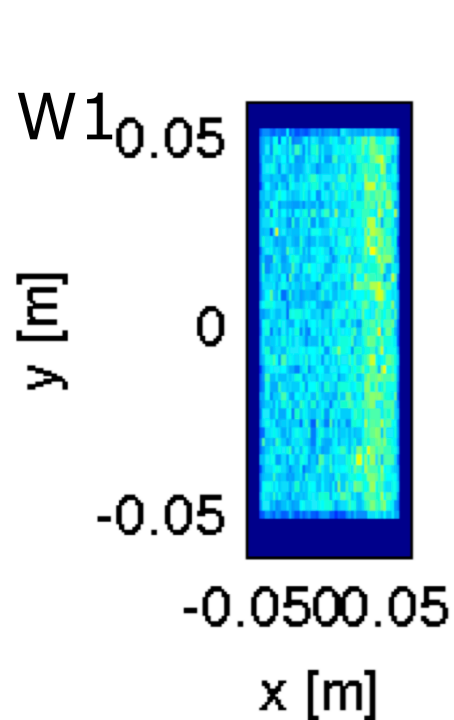


Analytic

Unfiltered  
"BIG" MCPL

"BIG" MCPL  
Geom filters  
in McStas instr

"Filtered" MCPL (E,neutr  
+geom filters  
in McStas instr



**50 sec**

**5.5 min**

**2.6 min**

**1.3 min**

Execution times...

ESS sources in McStas

# 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](#)