

Erik Knudsen, DTU Physics

Sources and Monitors part 2.

Sources: Source model overview

➤ **Mathematical:**

- *Source_simple.comp*
- *Source_div.comp*

➤ **Pulsed sources:**

- *ESS_butterfly.comp*
- *ESS_moderator.comp*
- *Moderator.comp*
- *SNS_source.comp (*)*
- *SNS_source_analytic (*)*
- *ViewModISIS (*)*
- *ISIS_moderator.comp (*)*

➤ **Reactors :**

- *Source_Maxwell_3.comp*
- *Source_gen.comp*
- *Source_gen4.comp*
- *Source_multi_surfaces.comp (*)*

➤ **I/O mechanisms:**

➤ **MCPL_input/output.comp**

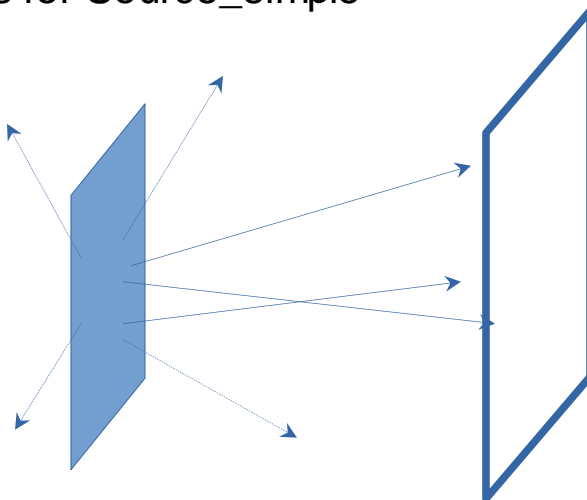
- *Virtual_input/output.comp*
- *Virtual_mcnp_ss_input/output.comp*
- *Virtual_tripoli4_input/output.comp*
- *Vitess_input/output.comp*

Sources: Source_Maxwell_3

```
COMPONENT source = Source_Maxwell_3(yheight=0.156, xwidth=0.126,  
Lmin=0.1, Lmax=9.0, dist=1.5, focus_xw = 0.025, focus_yh = 0.12,  
T1=150.42, I1=3.67E11, T2=38.74, I2=3.64E11, T3=14.84, I3=0.95E11)
```

Parameters from the PSI cold source

Initial position and direction: as for Source_simple



Sources: Source_Maxwell_3

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```
COMPONENT source = Source_Maxwell_3(yheight=0.156, xwidth=0.126,  
                                     Lmin=0.1, Lmax=9.0, dist=1.5, focus_xw = 0.025, focus_yh = 0.12,  
                                     T1=150.42, I1=3.67E11, T2=38.74, I2=3.64E11, T3=14.84, I3=0.95E11)
```

Parameters from the PSI cold source

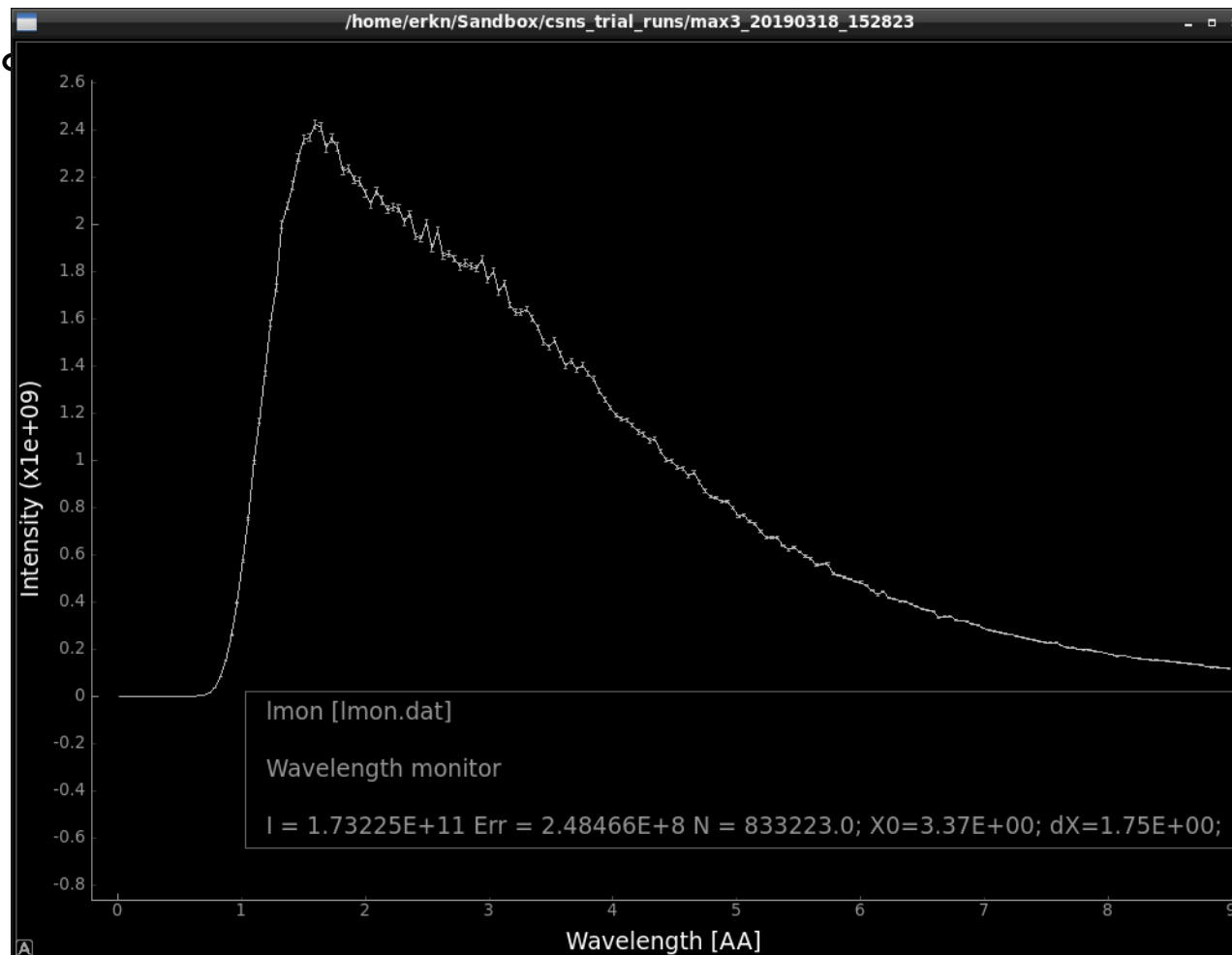
Intensity at a given wavelength drawn from a sum of (up to) 3
normalized Maxwellian distributions:

$$I(\lambda) = \sum I_i M(\lambda, T_i); \quad M(\lambda, T_i) = 2\alpha^2 \exp\left(\frac{-\alpha}{\lambda^2}\right) / \lambda^5 ;$$

$$\alpha = 949.0 K A A^2 / T_i$$

Sources: Source_Maxwell_3

COMPONENT source



26,
, focus_yh = 0.12,
3=14.84, I3=0.95E11)
in the PSI cold source

Sources: Source_Maxwell_3

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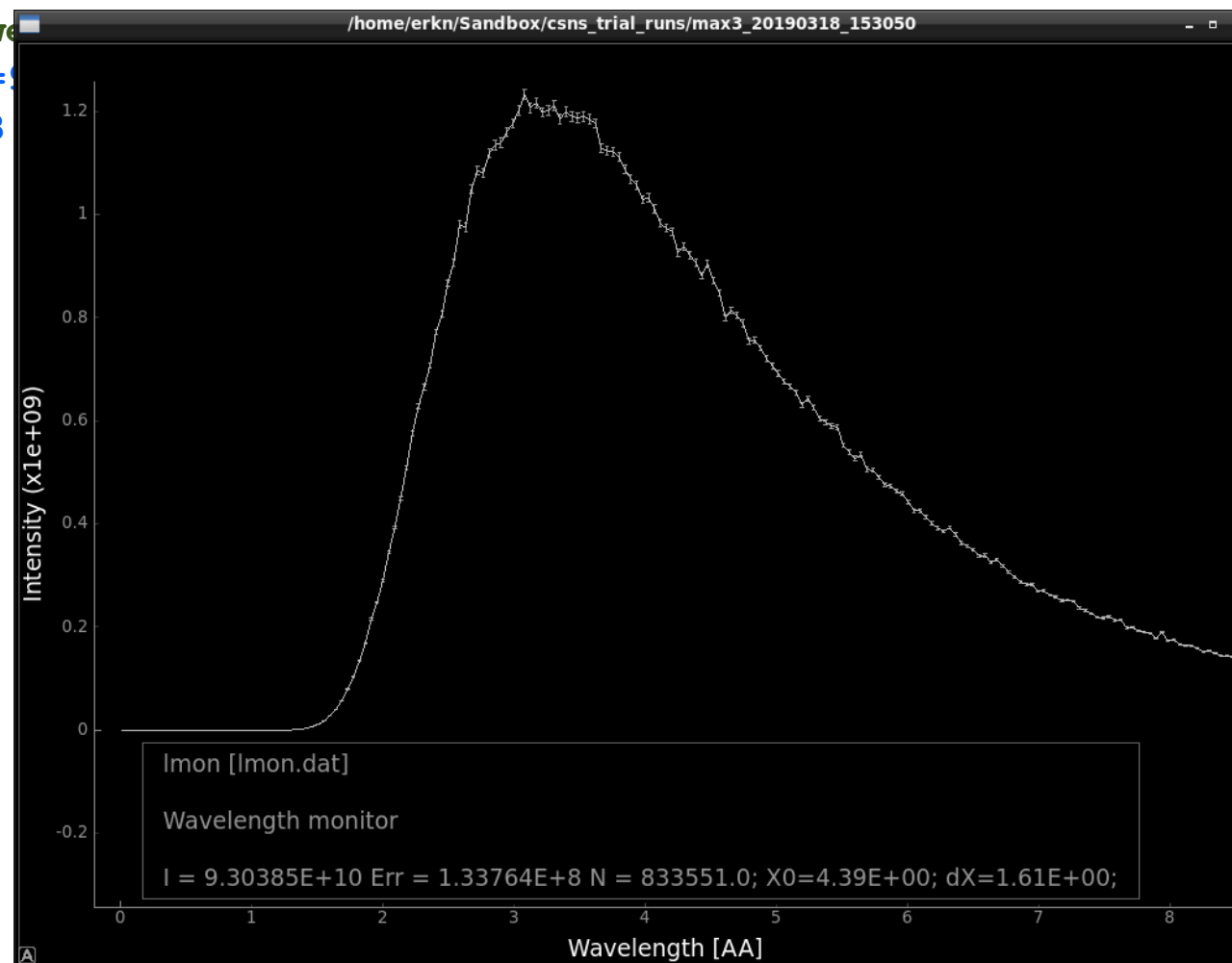
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```
COMPONENT source = Source_Maxwell_3
Lmin=0.1, Lmax=1000000
T1=150.42, I1=30000000000
```

Just for fun – let's see what happens if we remove the fast peak...



Input parameters

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

Name	Unit	Description	Default
size	m	Edge of cube shaped source (for backward compatibility)	0
yheight	m	Height of rectangular source	0
xwidth	m	Width of rectangular source	0
Lmin	AA	Lower edge of lambda distribution	
Lmax	AA	Upper edge of lambda distribution	
dist	m	Distance from source to focusing rectangle; at (0,0,dist)	
focus_xw	m	Width of focusing rectangle	
focus_yh	m	Height of focusing rectangle	
T1	K	1st temperature of thermal distribution	
T2	K	2nd temperature of thermal distribution	300
T3	K	3rd temperature of - - -	300
I1	1/(cm**2*st)	flux, 1 (in flux units, see above)	
I2	1/(cm**2*st)	flux, 2 (in flux units, see above)	0
I3	1/(cm**2*st)	flux, 3 - - -	0
target_index	1	relative index of component to focus at, e.g. next is +1 this is used to compute 'dist' automatically.	+1
lambda0	AA	Mean wavelength of neutrons.	0
dlambda	AA	Wavelength spread of neutrons.	0

Sources: Source_gen (Source_gen4)

```
COMPONENT source = Source_gen(yheight=0.156, xwidth=0.126,  
                                Lmin=0.1, Lmax=9.0, dist=1.5, focus_xw = 0.025, focus_yh = 0.12,  
                                T1=150.42, I1=3.67E11, T2=38.74, I2=3.64E11, T3=14.84, I3=0.95E11)
```

Almost the same as Source_Maxwell_3: but with optional flux-files as input.



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MCPL_input/output

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Reads/writes events directly from MCPL-format files:

"T. Kittelmann et. al., "", J. Phys. Comp., 2017

```
COMPONENT vout = MCPL_output(filename="voutput.mcpl",
                                doubleprec=1,polarisationuse=1,verbose=1)
```

```
AT (Xout,Yout,Zout) RELATIVE PREVIOUS
```

```
COMPONENT vin = MCPL_input(filename="voutput.mcpl",
                              polarisationuse=1,verbose=1)
```

```
AT (Xin,Yin,Zin) RELATIVE PREVIOUS
```

MCPL_input/output

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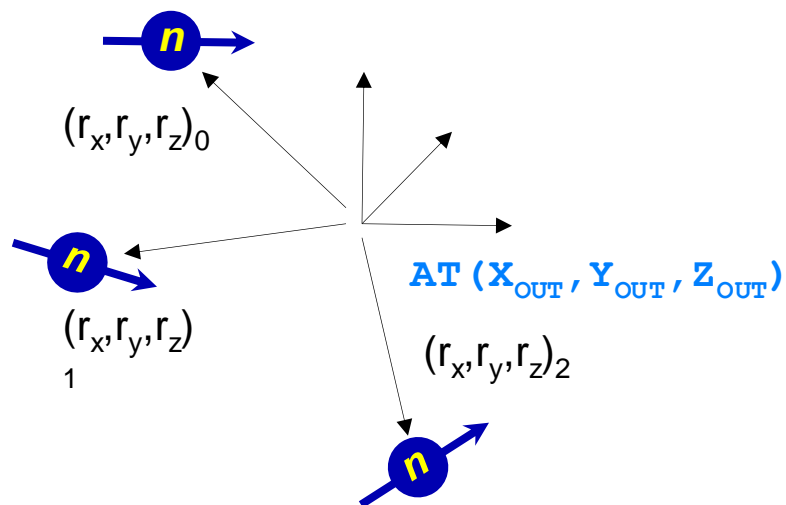
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Can include an Implicit Translation:

MCPL_output.comp



MCPL_input/output

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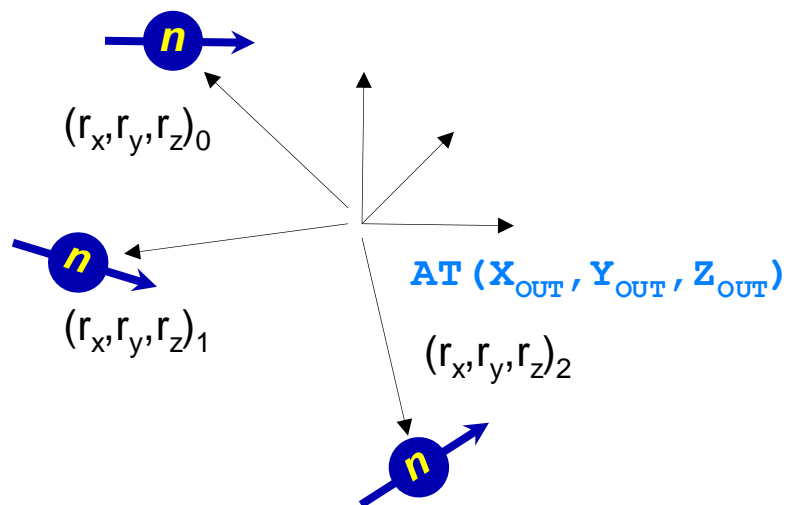
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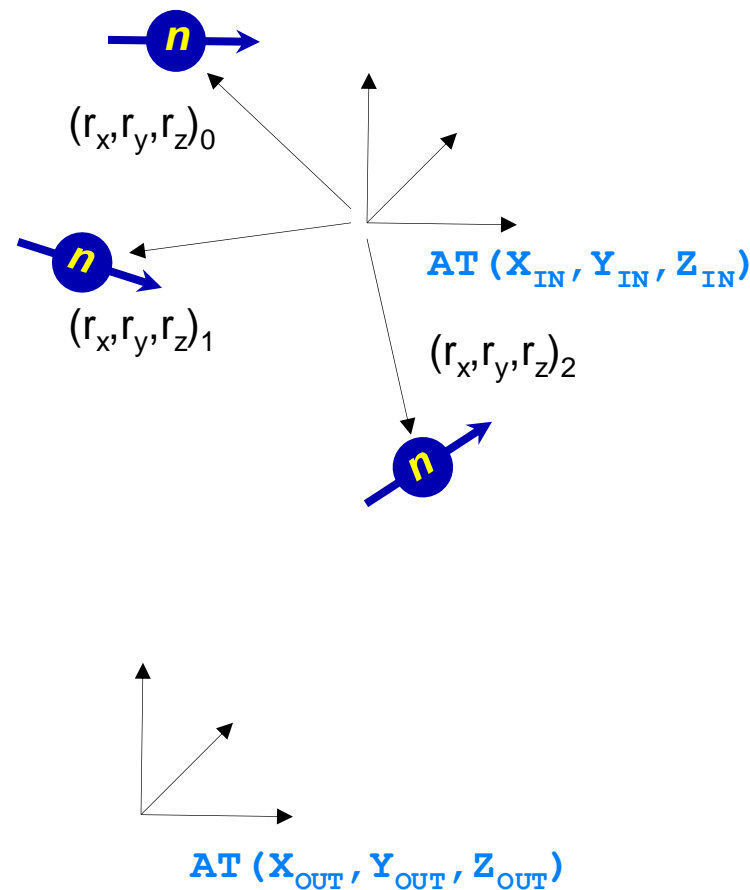
Can include an Implicit Translation:

MCPL_output.comp



BECOMES

MCPL_input.comp



Pulsed sources:

Simplest case:

Use a continuous source!

Model a source with given wavelength and spatial distribution

and

_____... an infinitely short pulse length. I.e. $t = 0$ for all neutron rays.

```
COMPONENT src = Source_simple(
    radius=0.05, lambda0=2.5, dlambda=1.5,
    focus_xw=0.1, focus_yh=0.1, dist=5 )
AT(0,0,0) RELATIVE origin
```

Pulsed sources:

Simplest case:

Use a continuous source!

Model a source with given wavelength and spatial distribution

and

_____ ... an infinitely short pulse length. I.e. $t = 0$ for all neutron rays.

```
COMPONENT src = Source_simple(
    radius=0.05, lambda0=2.5, dlambda=1.5,
    focus_xw=0.1, focus_yh=0.1, dist=5 )
AT(0,0,0) RELATIVE origin
EXTEND
%{
    t=0;
```

Pulsed sources:

Simplest case:

Use a continuous source!

Model a source with given wavelength and spatial distribution

and

... an infinite
COMPONENT

tron rays.

rad $\lambda=1.5$, $d\lambda=1.5$,
focus $=$, focus_yh=0.1, dist=5)

AT (0,0,0) **RELATIVE** origin

EXTEND

% {

t=0;

Or: Use a chopper
(see later)

Pulsed Sources: Moderator

A flat pulsed source with uniform energy spectrum:

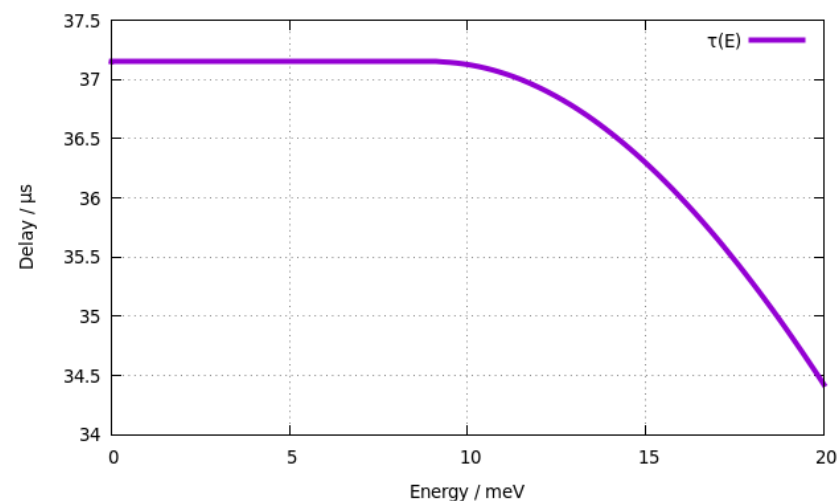
$$x \in U \left[-\frac{xwidth}{2}, \frac{xwidth}{2} \right] \quad y \in U \left[-\frac{yheight}{2}, \frac{yheight}{2} \right]$$

$$|v| = f(\lambda); \lambda \in U[L_{min}L_{max}]$$

Time structure is given by energy dependent probability density function:

$$f_t = \frac{1}{\tau} \exp \left(-\frac{t}{\tau} \right)$$

$$\tau = \begin{cases} t_0; & E < E_c \\ t_0 \left(\frac{1}{1 + \frac{(E - E_c)}{\gamma}} \right); & E \geq E_c \end{cases}$$





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Pulsed Sources: ESS_butterfly

- Analytic fits to MCNP-generated files.
- Specialized fits to each beamport.
- Fast and reasonably accurate.

Pulsed Sources: ESS_butterfly

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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

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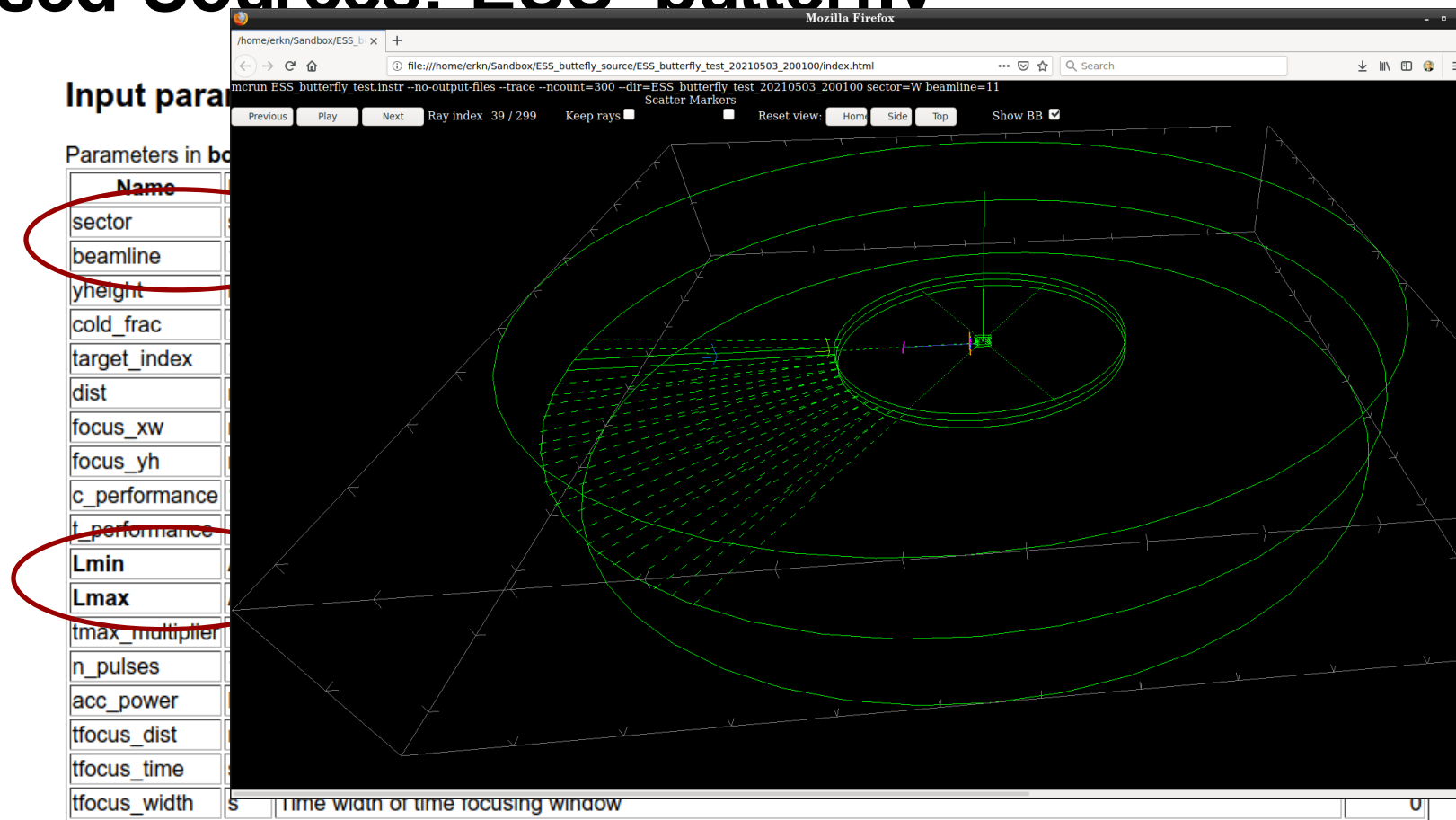
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Pulsed Sources: ESS butterfly

"W" - 11



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Pulsed Source

"W" - 11

Input parameters

Parameters in bold

Name	Unit
sector	str
beamline	1
yheight	m
cold_frac	1
target_index	1
dist	m
focus_xw	m
focus_yh	m
c_performance	1
t_performance	1
Lmin	AA
Lmax	AA
tmax_multiplier	1
n_pulses	1
acc_power	MW
tfocus_dist	m
tfocus_time	s
tfocus_width	s

Time width of time focusing window

0

McStas simulation window showing a 3D model of a synchrotron beamline. The window title is "Mozilla Firefox" and the address bar shows the file path: "file:///home/erkn/Sandbox/ESS_butterfly_source/ESS_butterfly_test...". The command line input is: "mcrun ESS_butterfly_test.instr --no-output-files --trace --ncount=300 --dir=ESS_butterfly_test_20210503_200100 sector=W beamline=11". The window displays a 3D model of a synchrotron beamline with various components like bending magnets, insertion devices, and a target. The beam path is shown as a series of green lines. The window also includes a "Previous" button, a "Play" button, a "Next" button, a "Ray index" display (39 / 299), a "Keep rays" checkbox, a "Scatter Markers" checkbox, and a "Reset view" button with options "Home", "Side", and "Top".

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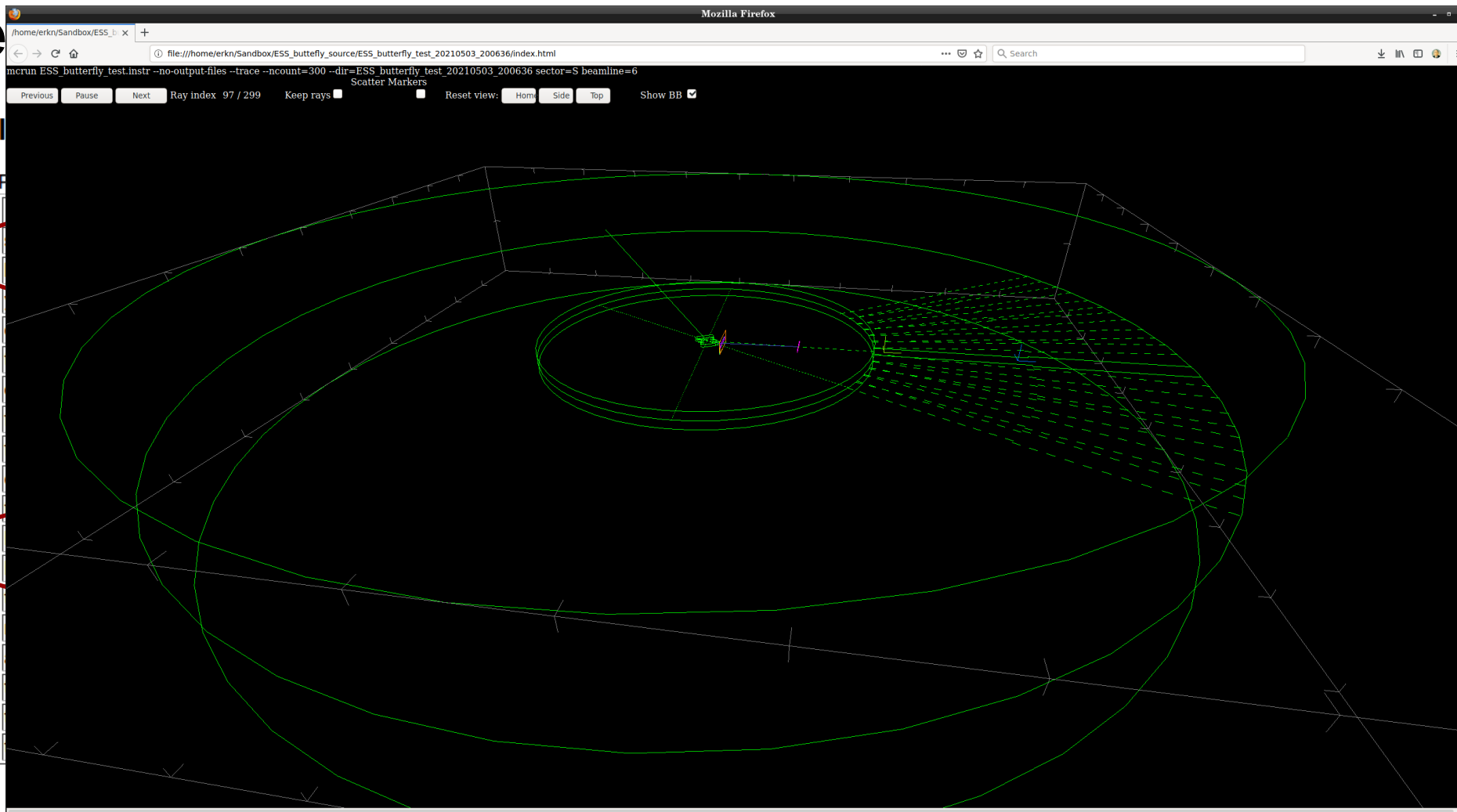


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Pulse

"S" - 6

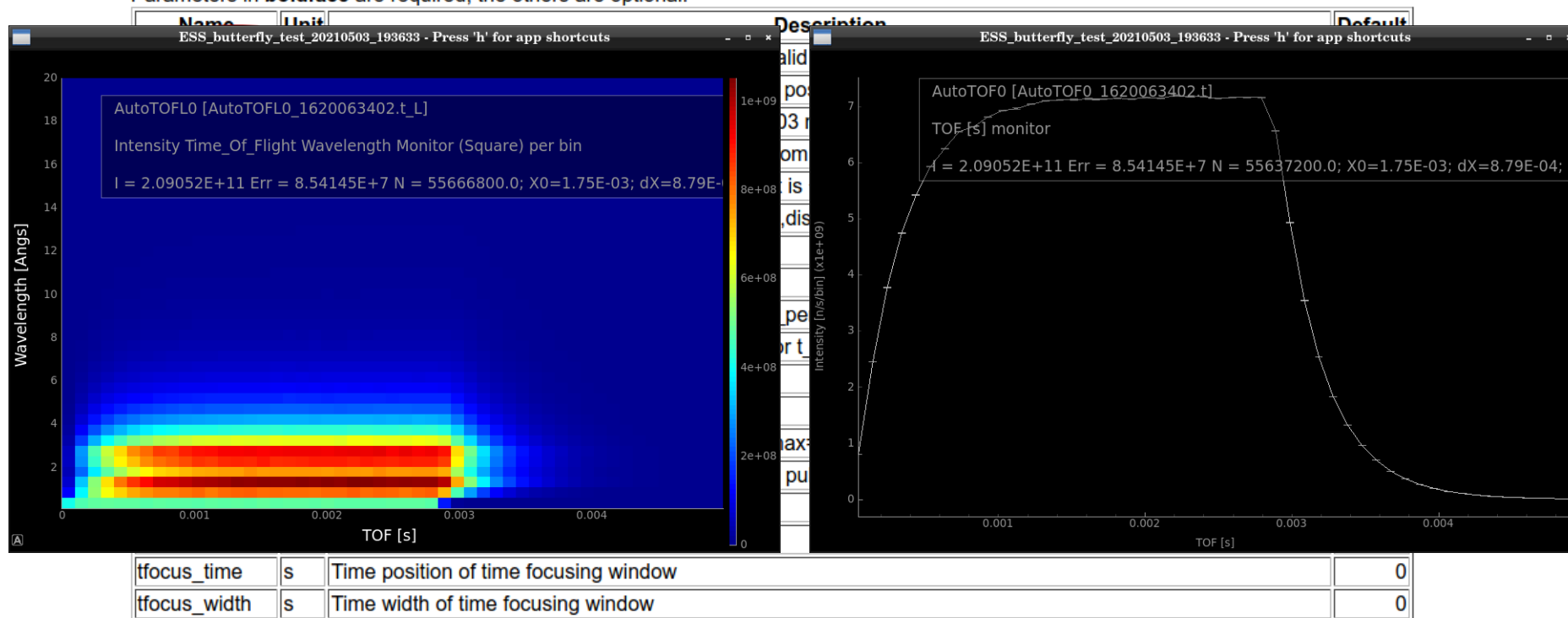


Pulsed Sources: ESS_butterfly

Input parameters

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

Example: N-1



Pulsed Sources: ESS_butterfly

n_pulses=3

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
tfocus_time	s	Time position of time focusing window	0
tfocus_width	s	Time width of time focusing window	0

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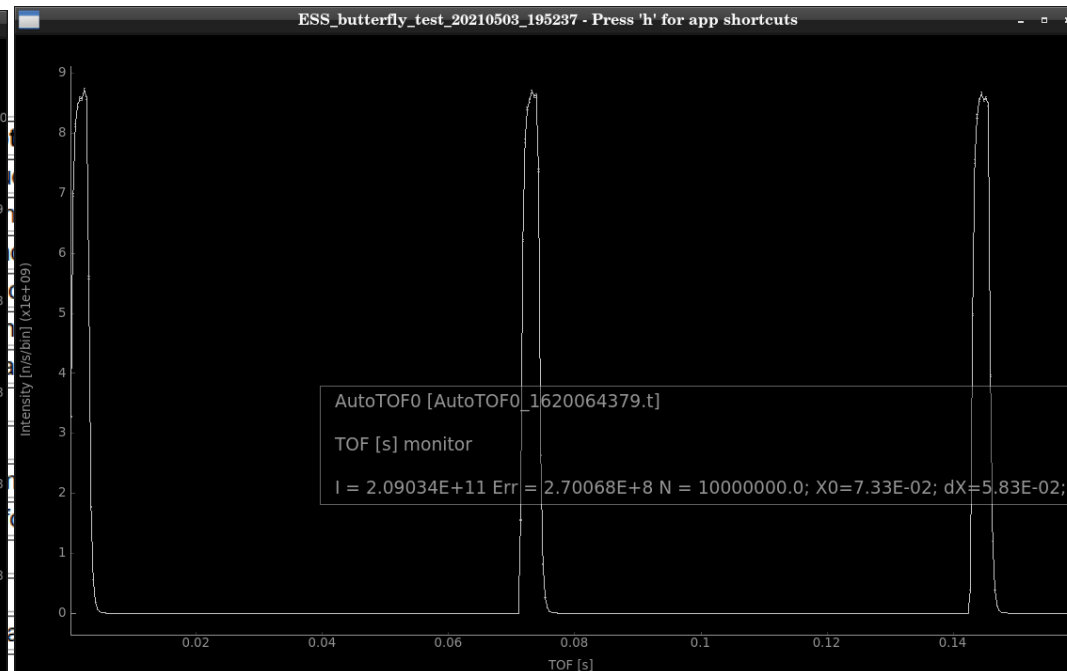
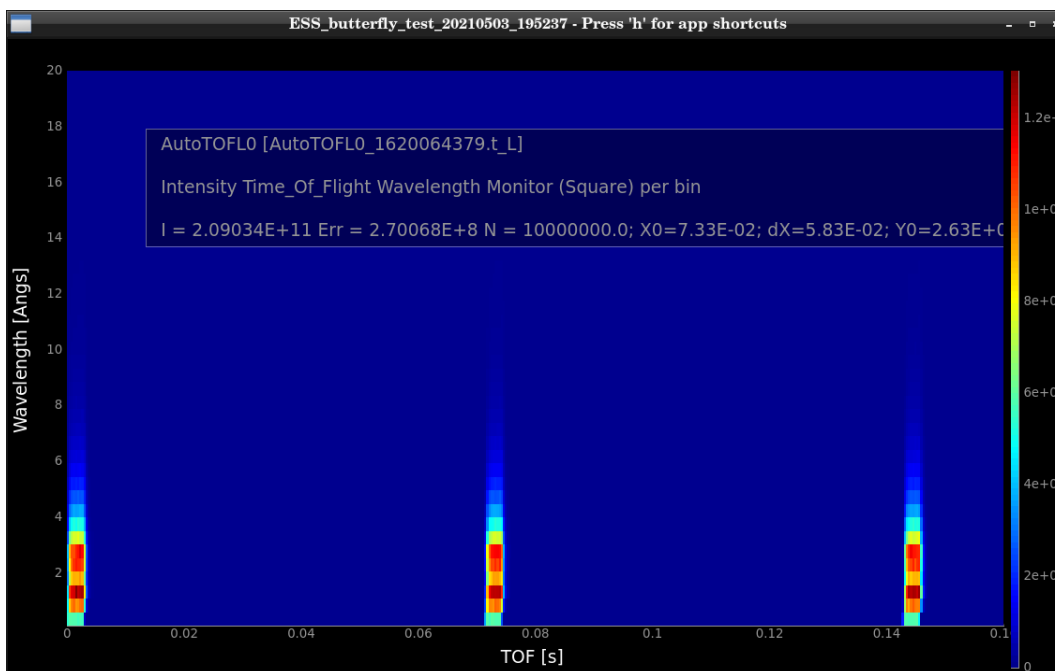
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Pulsed Sources: ESS_butterfly

n_pulses=3



n_pulses	3	Number of pulses simulated and created in pulse generator	
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





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Pulsed Sources: ViewModISIS

- Samples directly from tallies coming from e.g. MCNP target+moderator calculations.
- Data file supplied for each beam port at ISIS.

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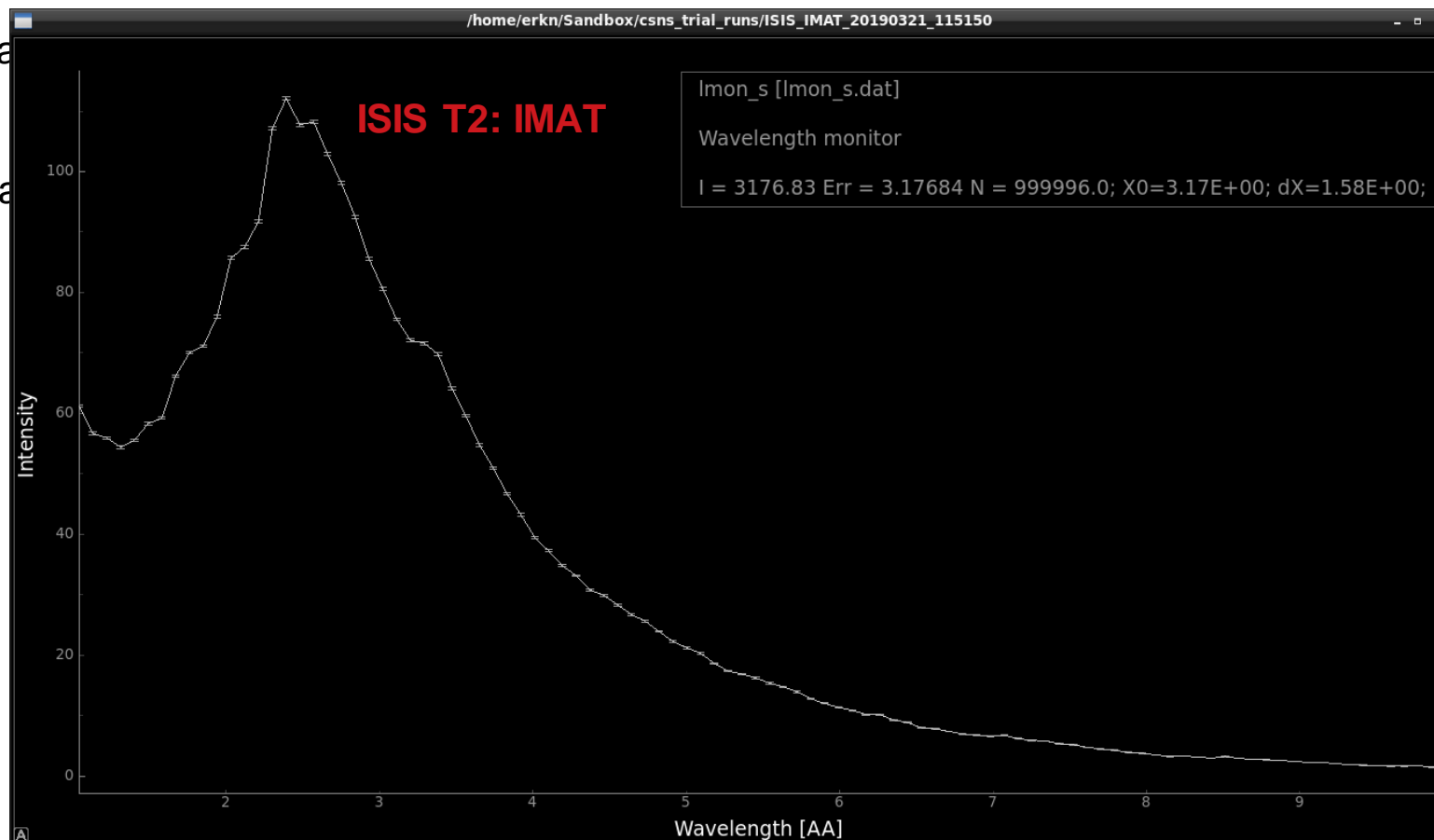
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Pulsed Sources: ViewModISIS

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Pulsed Sources: SNS_source

- Samples directly from tallies coming from e.g. MCNP target+moderator calculations.
- Originally from SNS but also used extensively at J-PARC
- Can be used (with the proper input files) to model CSNS, and likely also ISIS.

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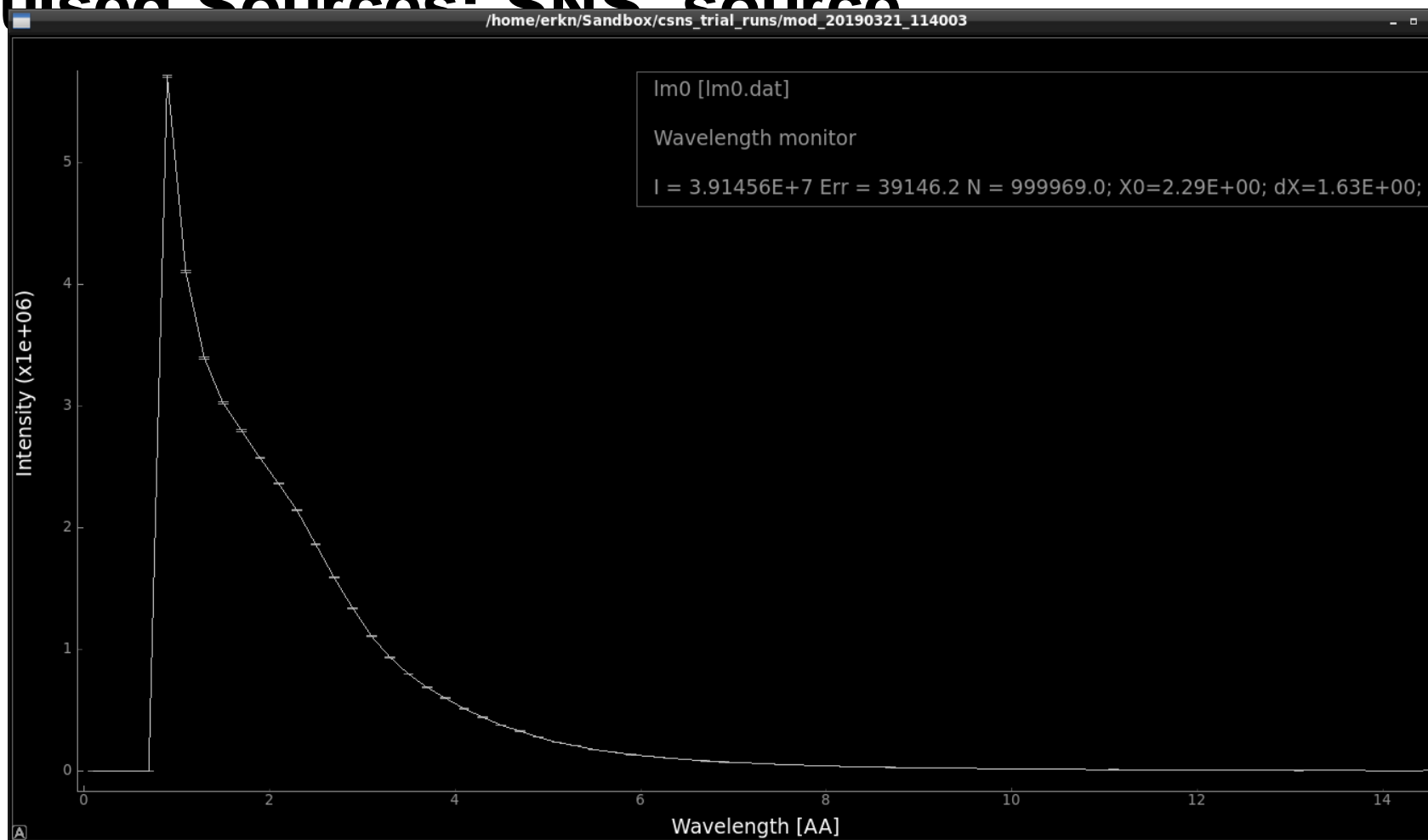
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Pulsed Sources: SNS source



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Pulsed Sources: SNS_source_analytic

- Samples from fits of Padé-functions to tallies from SNS_source.
- - Requires a complex fitting campaign
- + Much faster than SNS_source
 - + “Cleaner” distributions where statistics are sketchy
- Can be used (with the proper input files) to model CSNS-source.

Monitors (some)

1D

- ◆ L_monitor $\rightarrow I(\lambda)$
- ◆ TOF_monitor $\rightarrow I(t)$
- ◆ Hdiv_monitor $\rightarrow I(div.x)$
- ◆ MeanPolLambda $\rightarrow \langle \bar{P} \rangle(\lambda)$
- ◆ E_monitor $\rightarrow I(E)$

2D

- ◆ PSD_monitor $\rightarrow I(x, y)$
- ◆ PSD_monitor_4PI $\rightarrow I(\theta, \phi)$
- ◆ PolLambda_monitor $\rightarrow I(\bar{P}, \lambda)$
- ◆ Divergence_monitor $\rightarrow I(div.x, div.y)$
- ◆ DivPos_monitor $\rightarrow I(div.x, x)$

nD

- ◆ Monitor_nD \rightarrow
 $I(X)$
or $I(X, Y)$
or $Z(X, Y, Z)$
or ...



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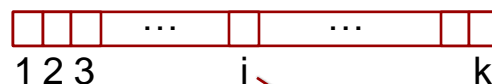
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Monitors: Quick examples

```
COMPONENT my_L_monitor = L_monitor(xwidth=0.2, yheight=0.2,  
                                     nL=20, filename="Output.L", Lmin=2, Lmax=10)
```

In a histogram sense

□ Imagine a histogram, e.g. $I(\lambda)$

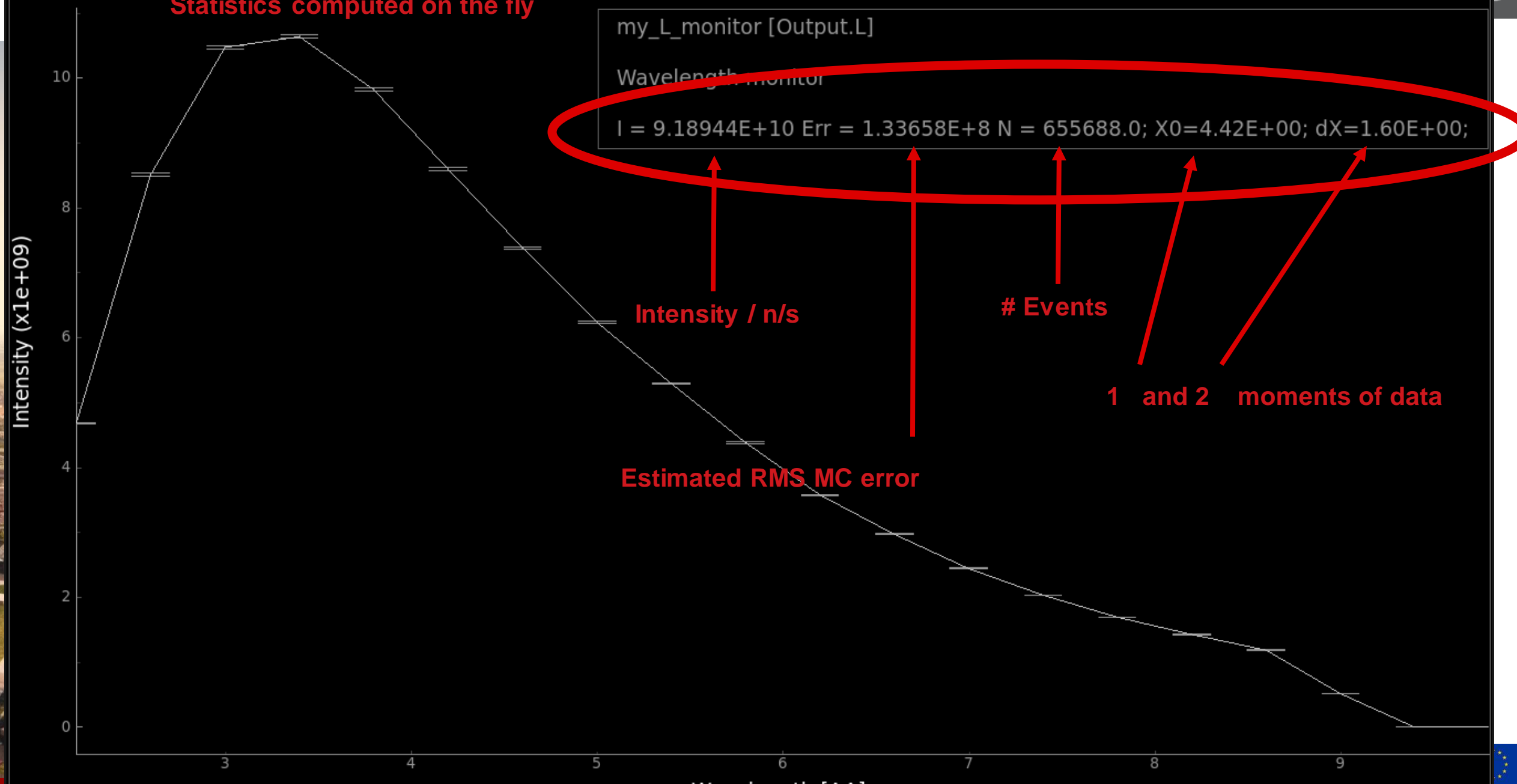


In bin i , N events each carrying a fractional intensity p_j so that

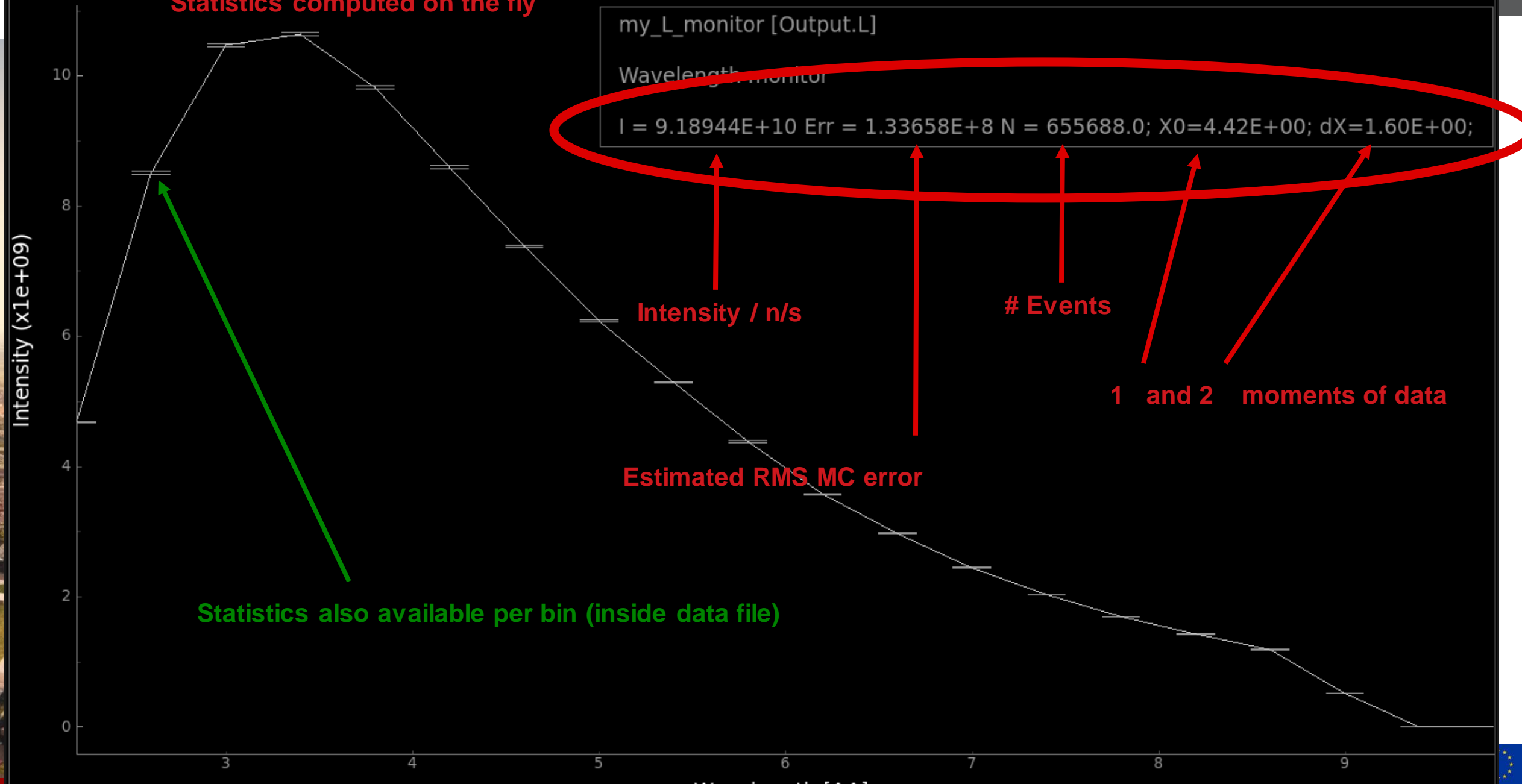
$$I = \sum_N p_j$$

□ The RMS variance over that set becomes our statistical error bar E

Statistics computed on the fly



Statistics computed on the fly



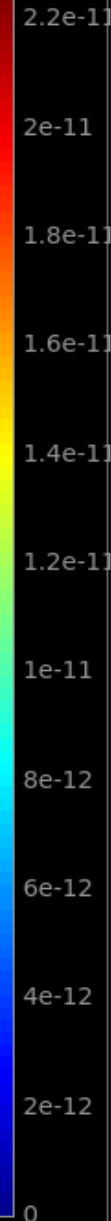
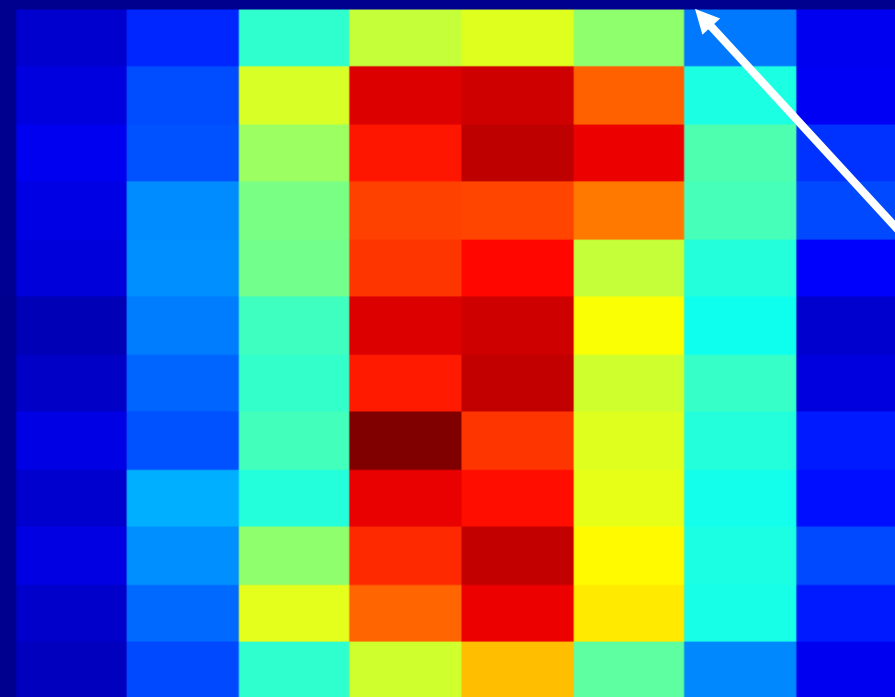
He3H [He3.psd]

PSD monitor

$I = 9.67067\text{E-}10$ Err = $6.31266\text{E-}12$ N = 25846.0; $X0=6.19\text{E-}02$; $dX=4.03\text{E-}01$; $Y0=2.07\text{E-}02$; $dY=1.43\text{E+}00$;

Y position [cm]

In 2D



1 and 2 moments

From "Virtual experiments - the ultimate aim of neutron ray-tracing simulations", K. Lefmann et al., Journal of Neutron Research 16, 97-111 (2008)

Let n be the number of neutron rays reaching the detector, and let the rays have (different) weights, w_i . The simulated intensity is then given by

$$I = \sum_{i=1}^n w_i. \quad (1)$$

The estimate of the error on this number is calculated in the McStas manual [1], and the standard deviation is approximated by

$$\sigma^2(I) = \sum_{i=1}^n w_i^2. \quad (2)$$

In real experiments, $w_i = 1$, whence we reach $I = n$ and $\sigma(I) = \sqrt{I}$ as expected (for counts exceeding 10). Let the virtual time be denoted by t . The simulated counts during this time becomes

$$C = tI, \quad (3)$$

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From "Virtual experiments - the ultimate aim of neutron ray-tracing simulations", K. Lefmann et al., Journal of Neutron Research 16, 97-111 (2008)

and its error bar estimate is

$$\sigma^2(C) = t^2 \sigma^2(I). \quad (4)$$

However, to simulate a realistic counting statistics, we must fulfill

$$\sigma_{VE}(C_{VE}) = \sqrt{C_{VE}}. \quad (5)$$

This is obtained by adding to (3) a Gaussian noise $E(\Sigma)$ of mean value zero and standard deviation Σ :

$$C_{VE} = tI + E(\Sigma). \quad (6)$$

The standard deviation for the VE becomes

$$\sigma_{VE}^2(C) = t^2 \sigma^2(I) + \Sigma^2. \quad (7)$$

Now, the requirement (5) allows us to determine Σ :

$$\Sigma^2 = tI - t^2 \sigma^2(I). \quad (8)$$

Since Σ^2 must remain positive, we reach an upper limit on t

$$t_{\max} = \frac{I}{\sigma^2(I)}. \quad (9)$$



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Sketch of an algorithm...

1. On a given McStas histogram
2. For the non-zero bins, calculate

$$t_{\max} = \frac{I}{\sigma^2(I)}.$$

The *smallest* t_{\max} defines the “maximal counting time” allowed by your statistics

3. Preferably a “background” should be added - use a “known experimental value” or an estimate...



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Monitor_nD

A general monitor for 0D/1D/2D records

The all-in-one , swiss-army-knife of monitors

***Monitor_nD** can have almost any shape, and record any requested standard quantities*



Monitor_nD

A general monitor for 0D/1D/2D records

Examples

```
COMPONENT MyMon = Monitor_nD( xwidth = 0.1, yheight = 0.1, zdepth = 0,  
    options = "intensity per cm2 angle,limits=[-5 5],  
    bins=10,with borders, file = mon1")
```

options = "banana, theta limits=[10,130], bins=120, y"

options = "multiple kx ky kz, auto abs log t, and list all neutrons"



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Monitor_nD

... or monitor just about anything:

```
COMPONENT MyMon = Monitor_nD(xwidth = 0.1, yheight = 0.1,  
    user1=age, username1="Age of the Captain [years]",  
    options="user1, auto")
```



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Exercise 2:

Head over to the github site and continue the exercise we started before:

https://github.com/McStasMcXtrace/Schools/tree/master/ISIS_April_2021/Tuesday_April_13th/2_Component_Basics/Exercise/

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