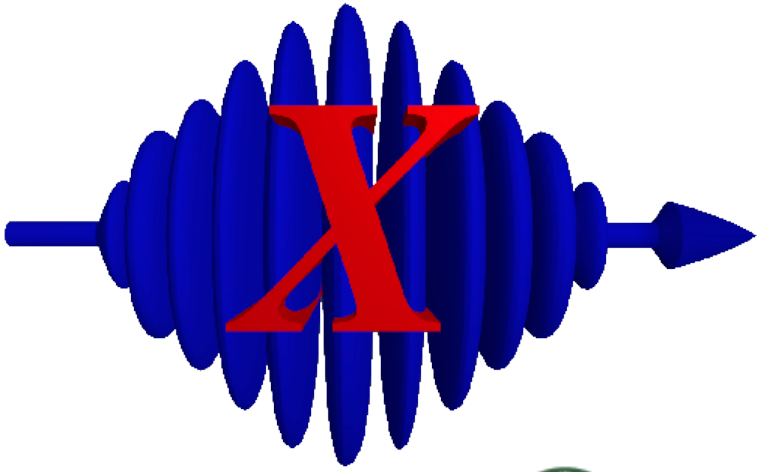
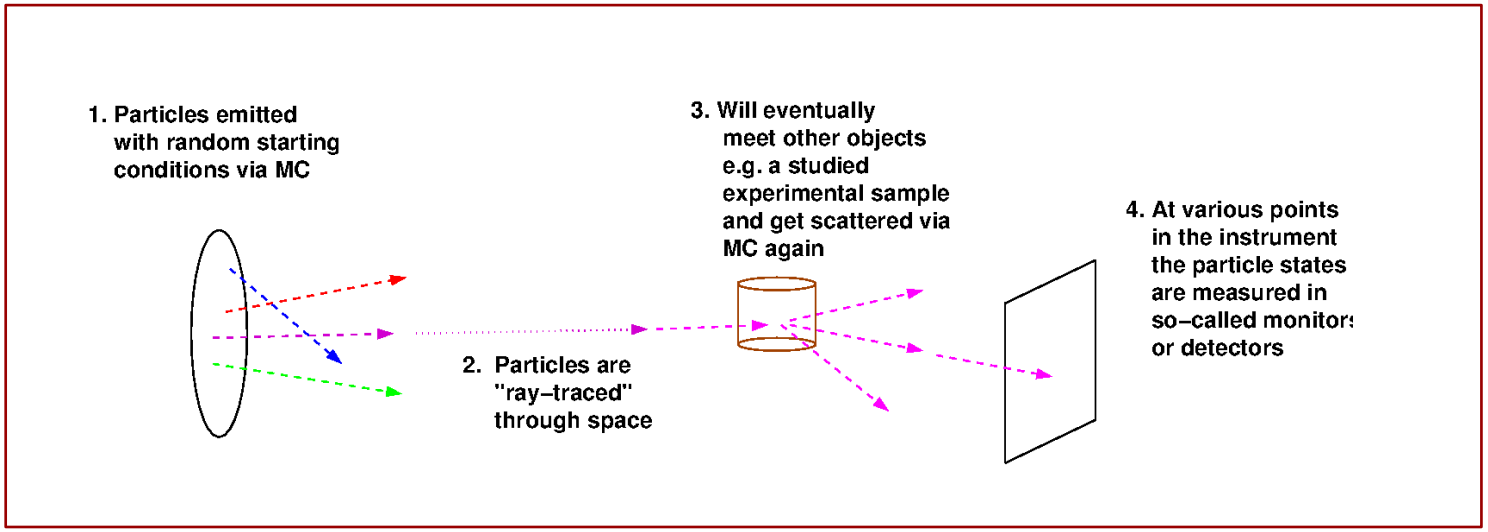
McXtrace



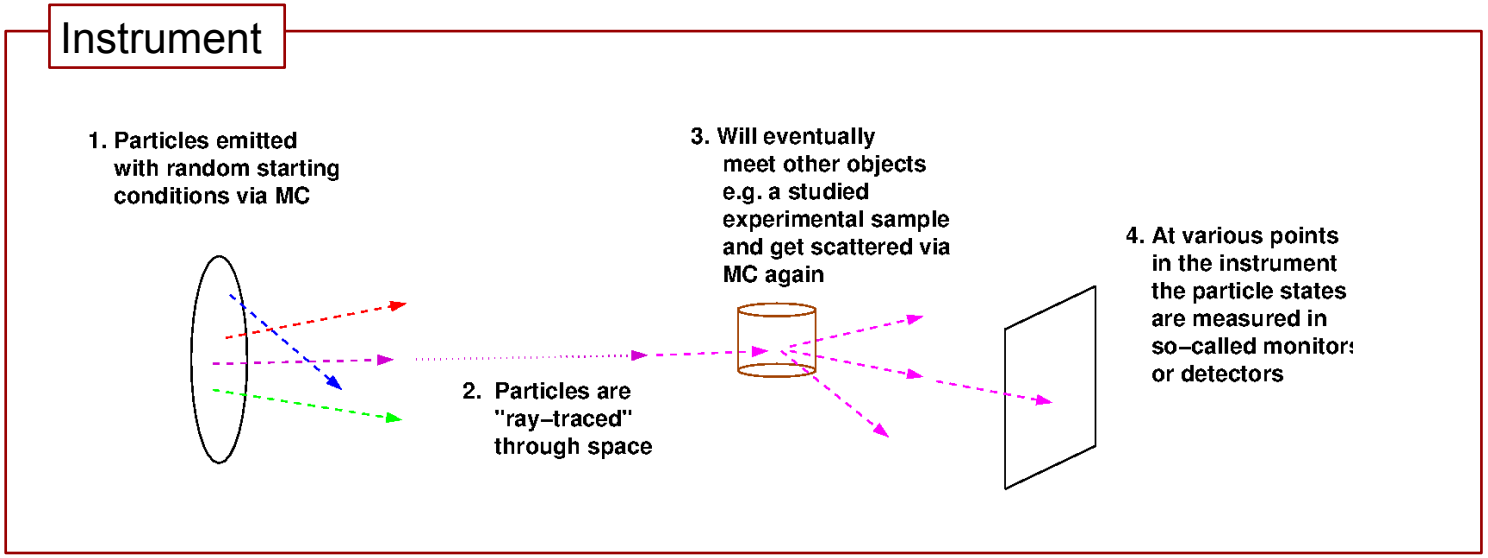
McXtrace components and instruments

Peter Willendrup (pkwi@fysik.dtu.dk)

In the big picture, McXtrace is this…

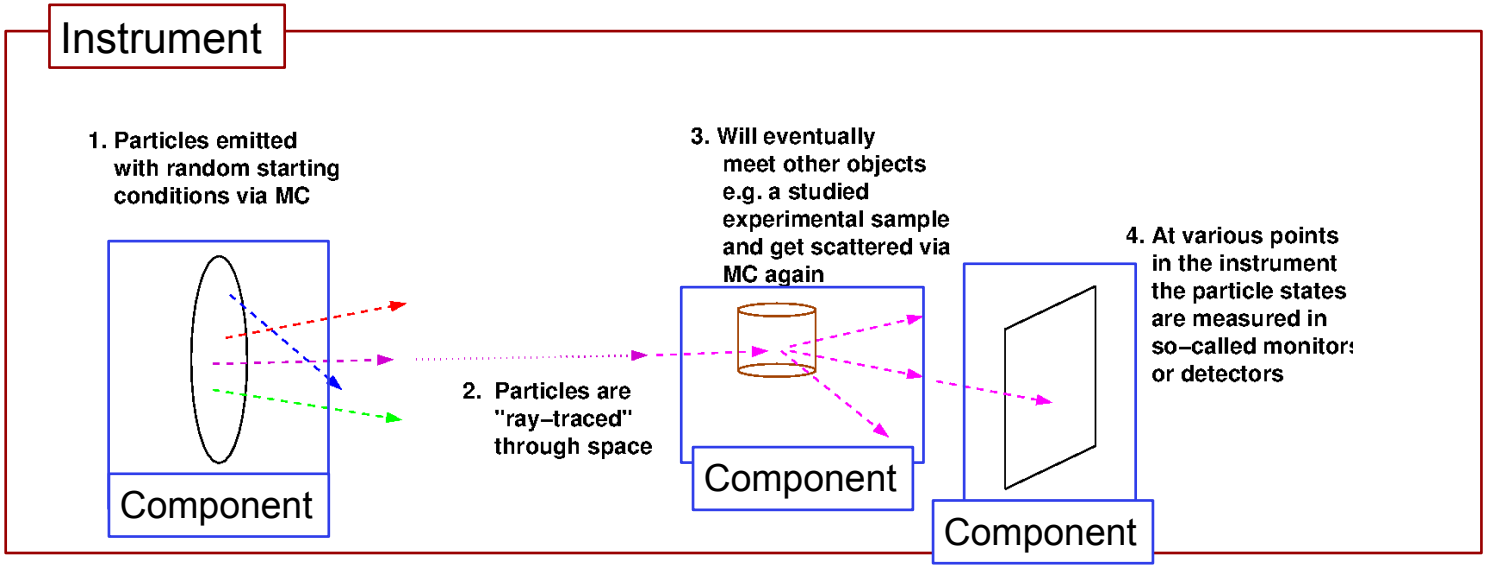


In the big picture, McXtrace is this…



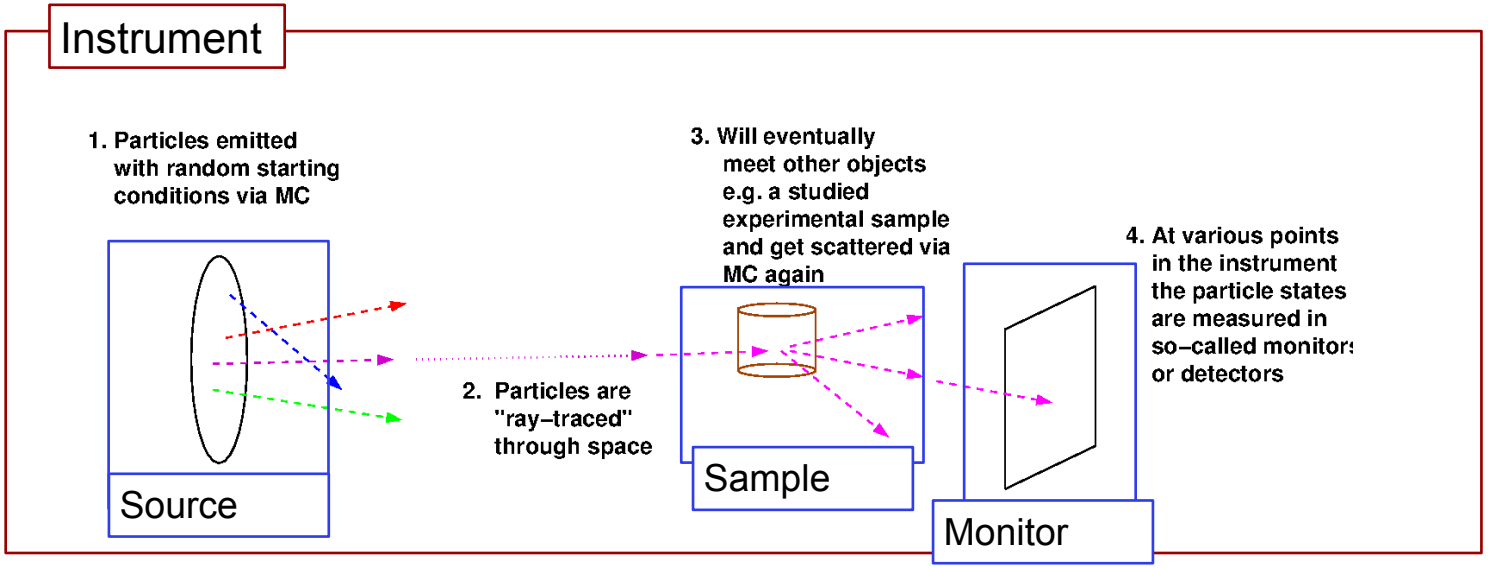
The instrument defines our “lab coordinate system”

In the big picture, McXtrace is this…



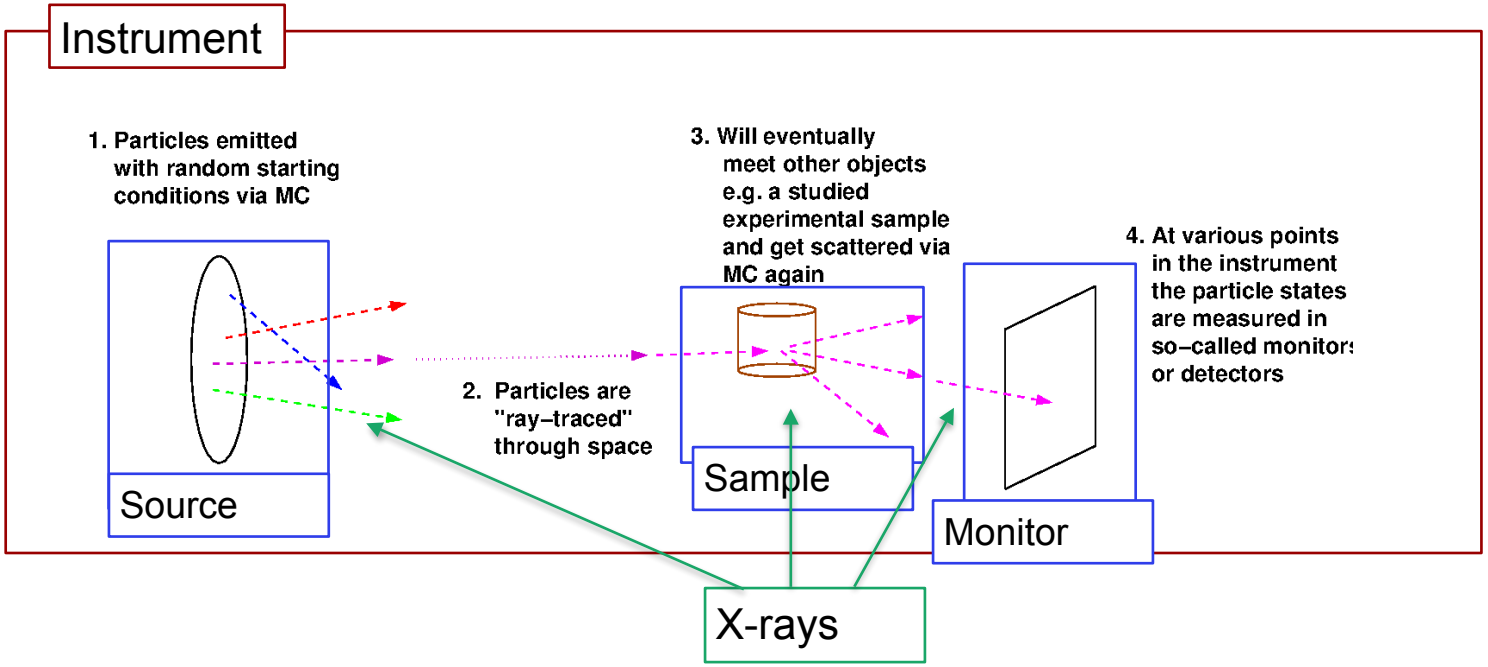
The instrument defines our “lab coordinate system”
The components define devices or features available in our instrument

In the big picture, McXtrace is this…



The instrument defines our “lab coordinate system”
The components define devices or features available in our instrument
- they have different function

In the big picture, McXtrace is this…



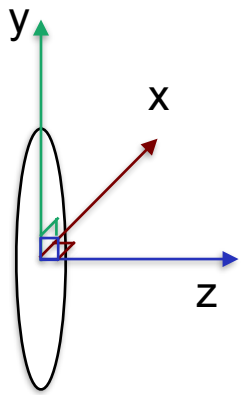
The instrument defines our “lab coordinate system”

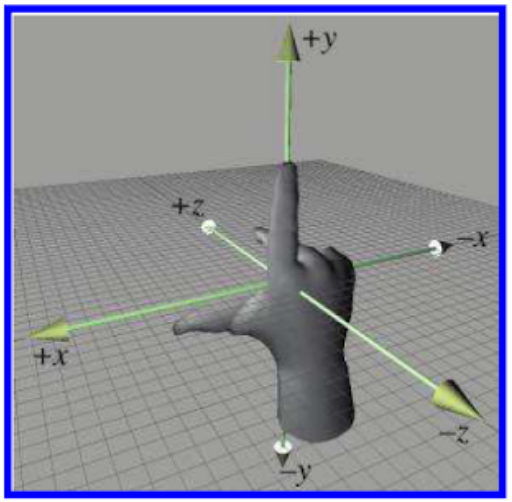
The components define devices or features available in our instrument - they have different function

X-ray photons particles are passed on from one component to the next, changing state under way

Placing components - source

- One of the first components in your instrument is typically a source, which has a coordinate system like this….



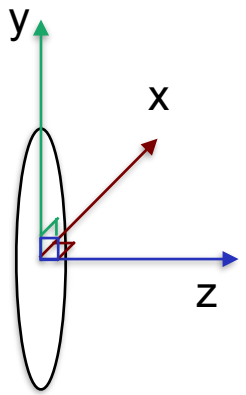


Right-handed coordinate system

- z is along X-ray beam direction
- y is vertical
- x at an angle of 90° wrt. z,y

Placing components - source

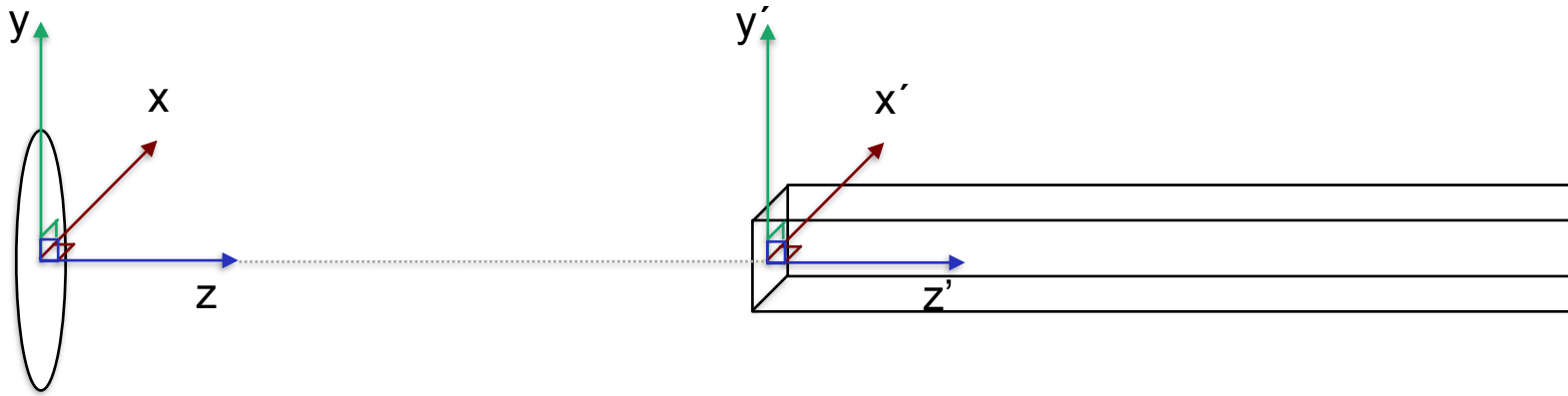
- Often the source coordinate system coincides with the “lab” coordinate system, denoted ABSOLUTE in McXtrace language, i.e.



- COMPONENT Source = Source_flat(…)
  AT (0,0,0) ABSOLUTE

Placing further components - RELATIVE

Placing further components is done by order of
1. **Location, i.e**

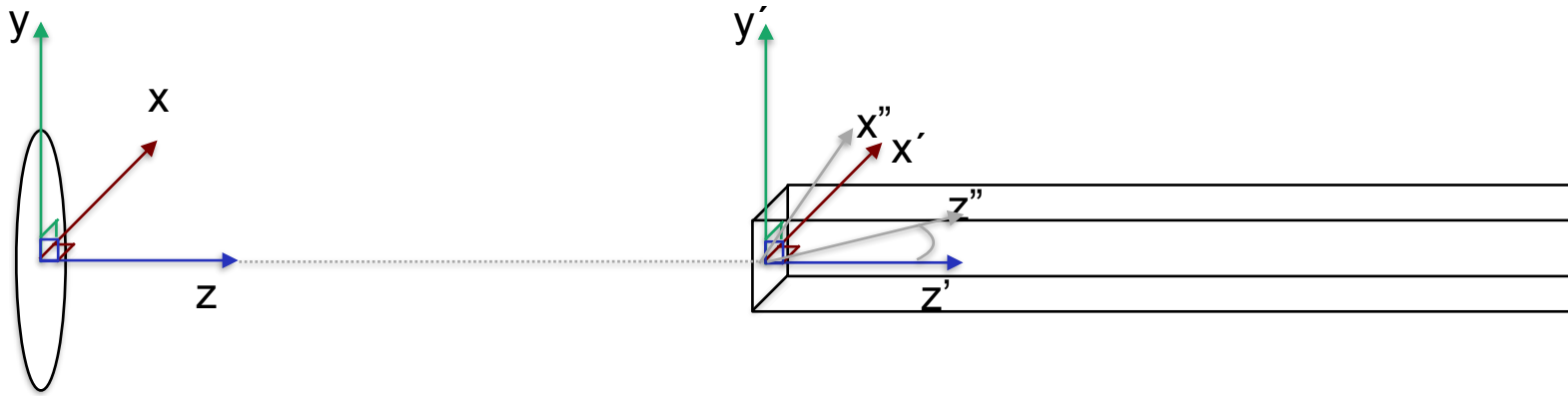


COMPONENT Source = Source_flat(…)
AT (0,0,0) ABSOLUTE

COMPONENT Capillary = Capillary(…)
AT (0,0,1) RELATIVE Source

Placing further components - RELATIVE

Placing further components is done by order of
2. **Rotation, i.e**



COMPONENT Source = Source_flat(…)
AT (0,0,0) ABSOLUTE

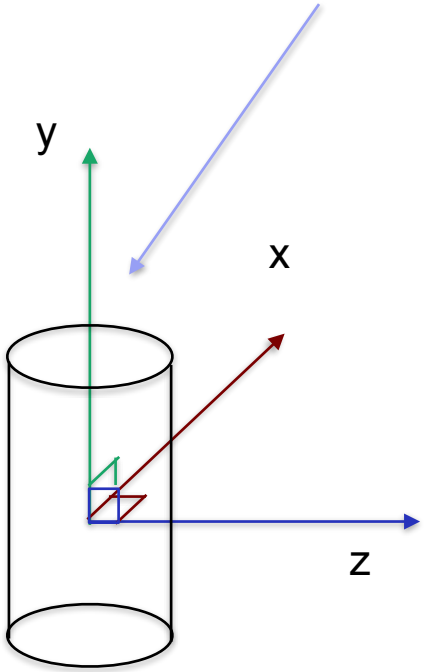
COMPONENT Capillary = Capillary(…)
AT (0,0,1) RELATIVE Source
ROTATED (0,0.1,0) RELATIVE Source

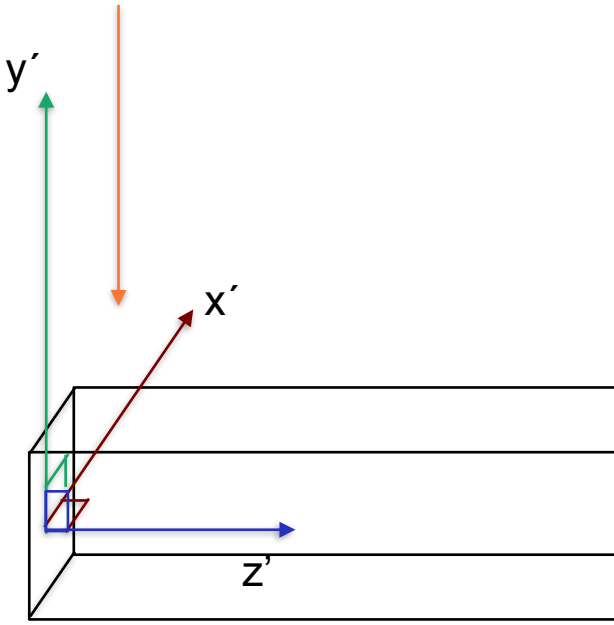
(Reference labels can also be PREVIOUS or PREVIOUS+1 etc.)

Note : AT and ROTATED can refer to different reference points and thus decoupled.

Components often have their origin at the centre of mass,
i.e. for samples … but not for e.g. Capillary

Placing further components is done by order of
2. **Rotation, i.e**



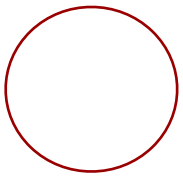


COMPONENT Sample = Some_sample(…)
AT (0,0,0) [RELATIVE] ABSOLUTE

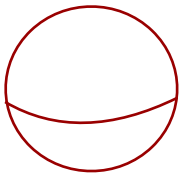
Generally speaking, the component author can choose
the meaningful coordinate system for the given problem!
- The McXtrace system takes care of the transformation between them….

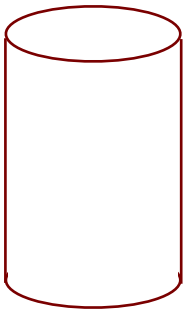
Component geometries are typically simple objects… But some have polygon-description of the surface

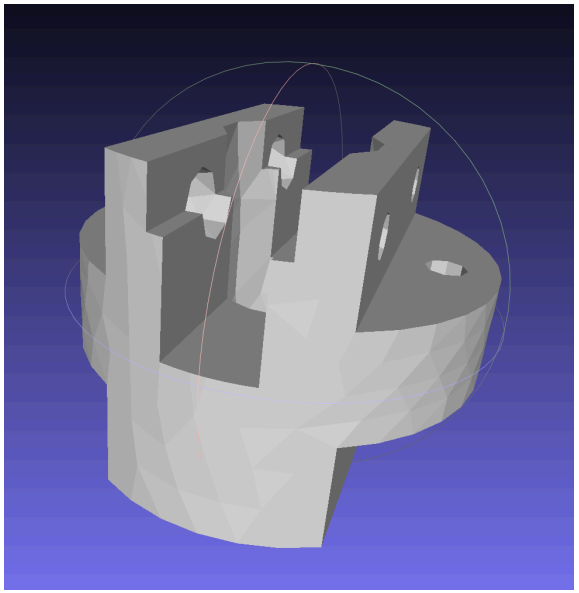
2D



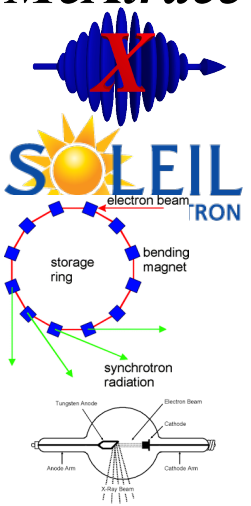
3D





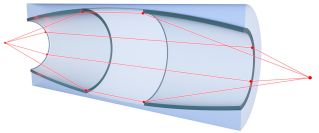


Component classes



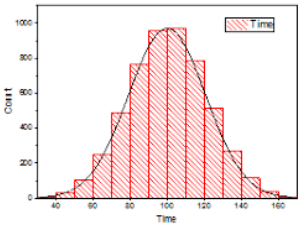
- Sources - these define MC starting conditions / “inject” rays to our simulation

- Optics - used to tailor properties of the X-ray beam
  - Examples are mirrors, capillaries, lenses, zone-plates, choppers, collimators, slits, …



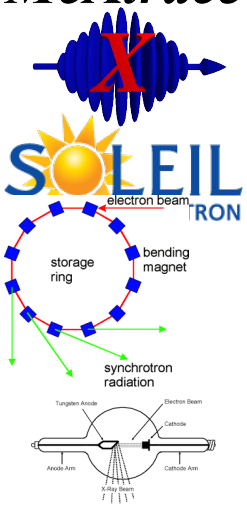
- Samples - “matter” of some form
  - Powders, single crystals, liquids, micelles in solution, reflecting surfaces…

- Monitors - may probe the state of the X-ray beam and store histograms / event lists



- Misc, obsolete
  - “Other stuff” and “Old stuff”

Component classes



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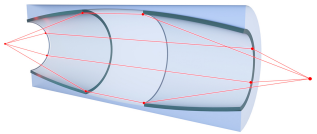

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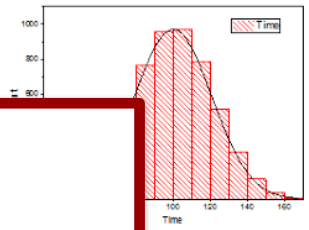


- Misc, obsol
  - “Other

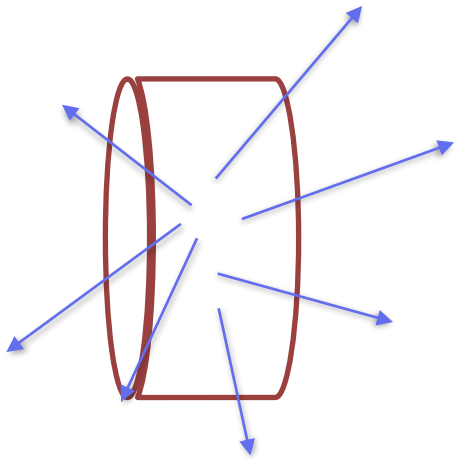
Common to all components:

They set, manipulate/interact with

or measure the **state of the X-ray** (ray)

Sources, e.g. rotating anode

- To first order emit uniformly into 4π steradian



Sources, e.g. rotating anode

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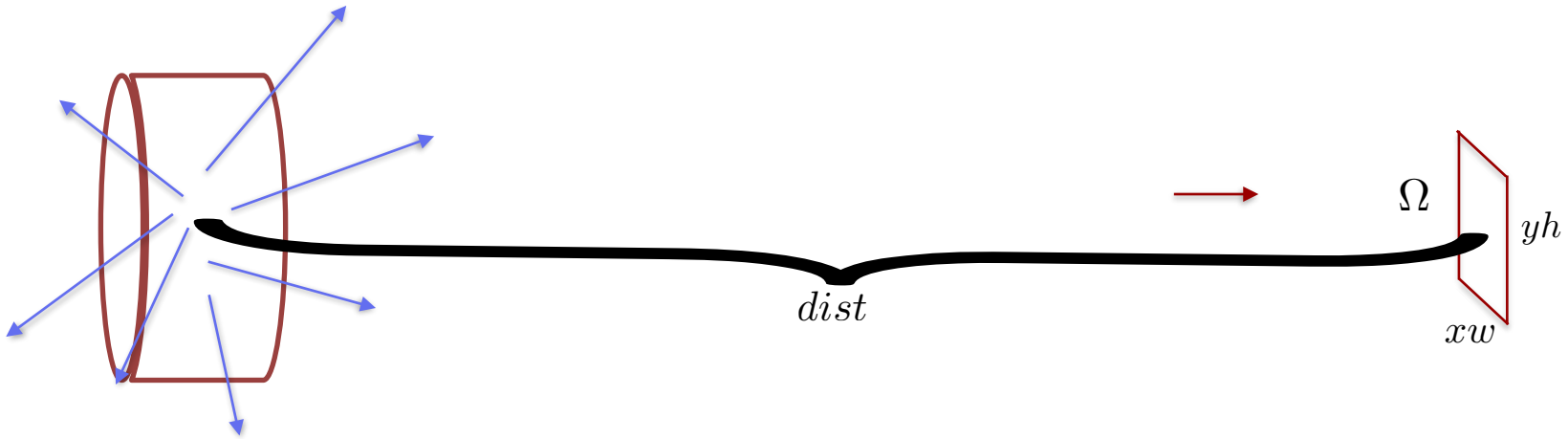
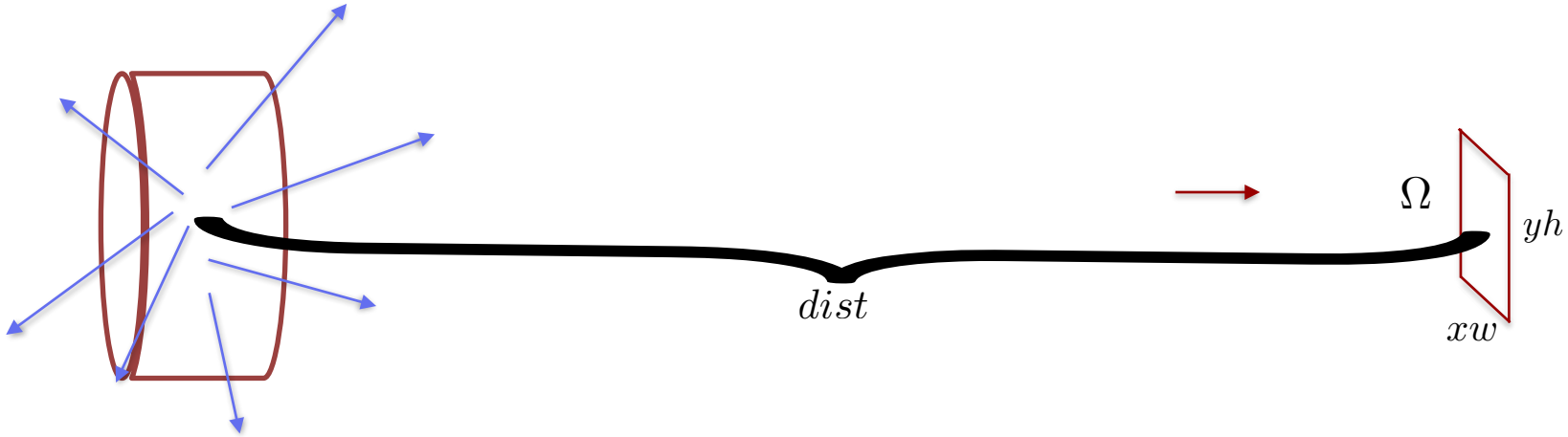


- Generally we are intersted in sending the input to an aperture, characterised by a certain solid angle Ω, often corresponding to a rectangle xw x yh at a distance $dist$ from the source

Sources, e.g. rotating anode

- The emmission intensity into our chosen solid angle Ω can be a function of wavelength, time (pulsed sources) and possibly point of origin on the source surface (e.g. for partially coherent descriptions).



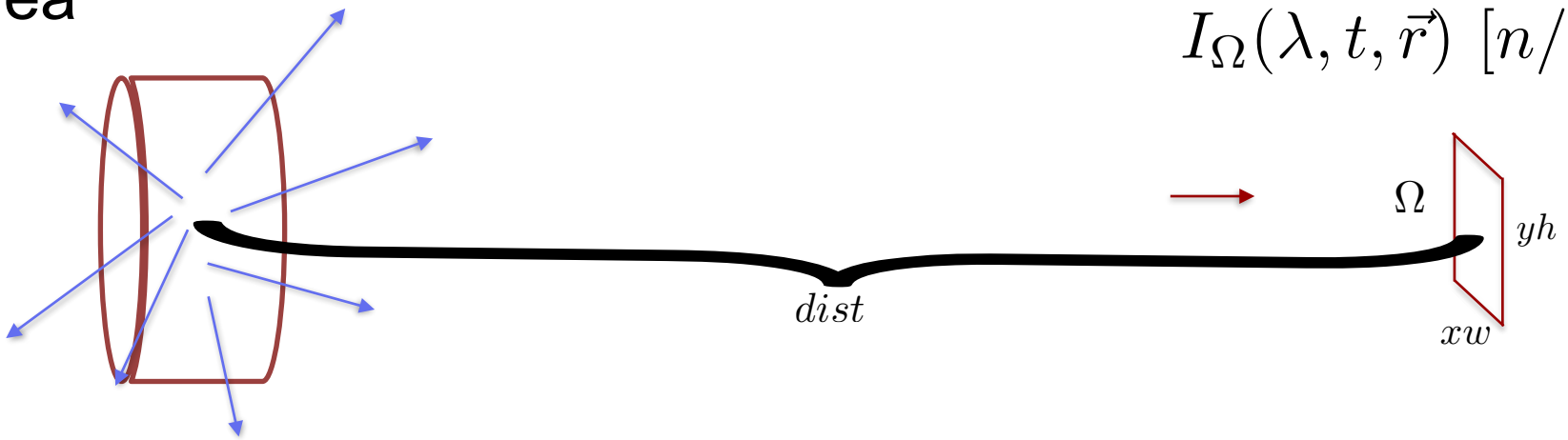
- The emission of particles into the solid angle Ω is in fact an integration and leads to a simulated "intensity" of $I_\Omega\ [n/s]$.
- In McXtrace, that integrated intensity is partitioned over a given set of particle *rays* referred to as **ncount**, **-n** or **--ncount**
- The default **ncount** is 1e6 rays

$$I(\lambda)\ [n/s/str]$$
$$I(\lambda, t)\ [n/s/str]$$
$$I(\lambda, t, \vec{r})\ [n/s/str]$$

Sources, e.g. rotating anode

- Our rays are emitted randomly, sampling Ω and all variables of the source “spectrum”, i.e. wavelength, time and area

$$I_\Omega(\lambda, t, \vec{r}) \ [n/s]$$



- assigning ray weights p such that

$$\sum_{j=1}^{\text{ncount}} p_j = \int_{d\lambda, dt, d\vec{r}} I_\Omega(\lambda, t, \vec{r})$$

X-ray (rays) in McXtrace - what are they?

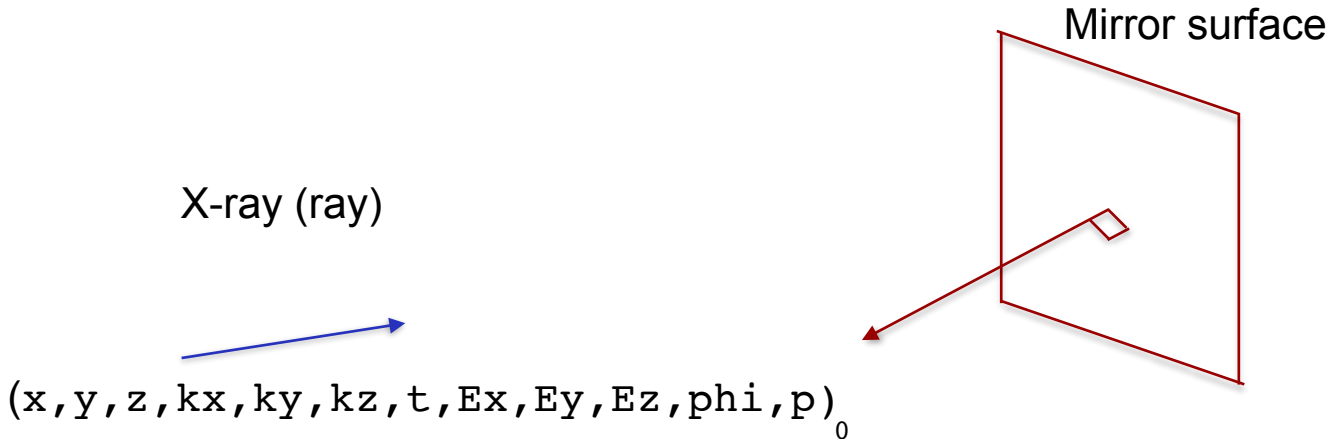
X-ray package:

Weight (p), # photons (left) in the package
Coordinates (x,y,z)
Wavevector (k_x,k_y,k_z)
Polarization (E_x,E_y,E_z)
Phase (ϕ)
Time(t)

- Defining the ray starting conditions imply setting:
  - The **starting point** on the surface, i.e. $\vec{r}$ (in the code variables `x,y,z`)
  - The **direction** into Ω and our λ / k (in the code variables `kx,ky,kz`)
  - The **starting time** (in the code the variable `t`)
  - The initial **intensity** / weight of the X-ray ray (in the code the variable `p`)
  - If needed the initial
    - **Electric field polarisation** (in the code the variables `Ex,Ey,Ez`)
    - X-ray phase (in the code the variable phi)

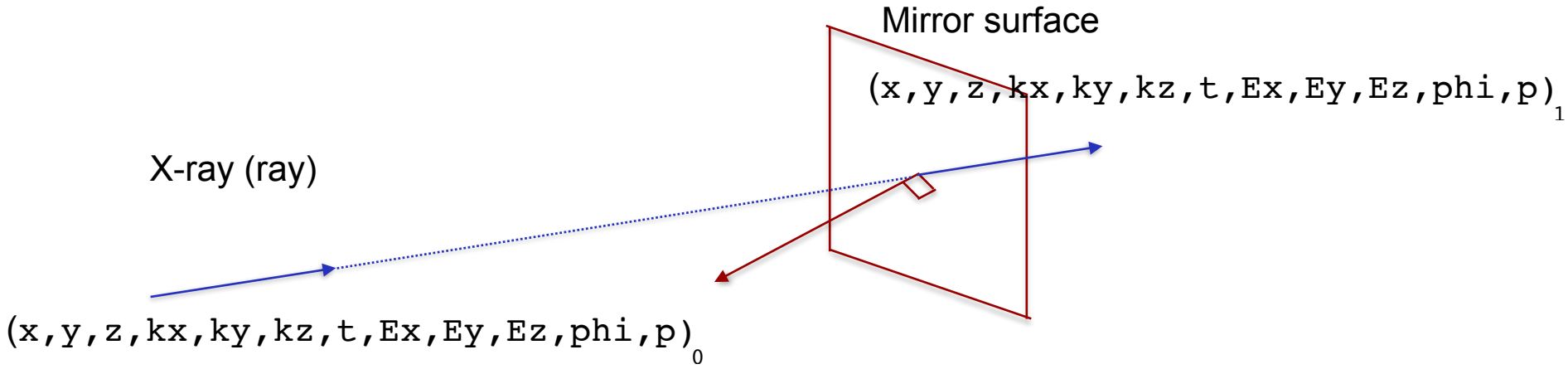
X-ray / matter interaction 1: reflecting surface

- 1 starting situation



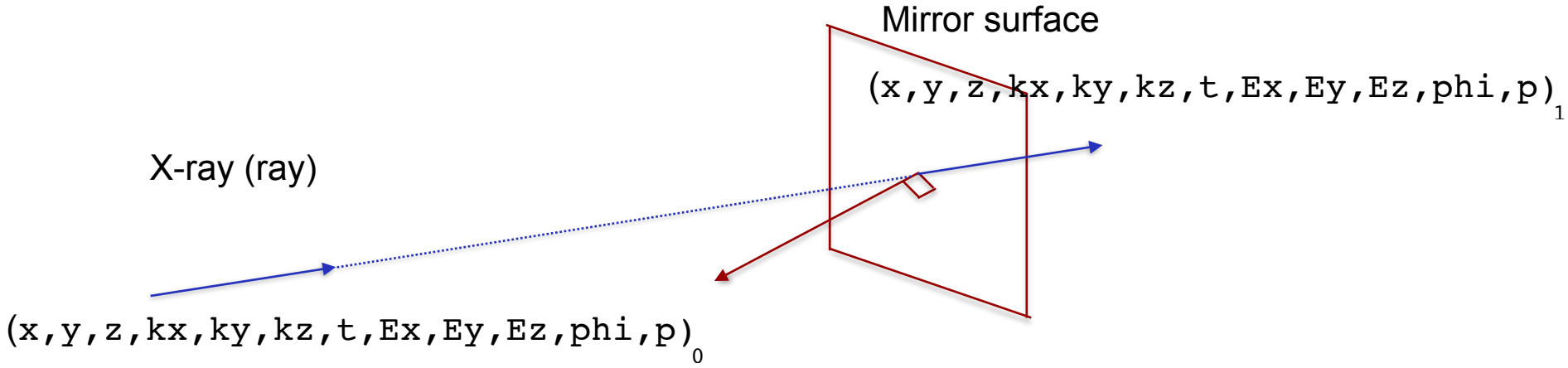
X-ray / matter interaction 1: reflecting surface

- 2. Propagate to the mirror surface



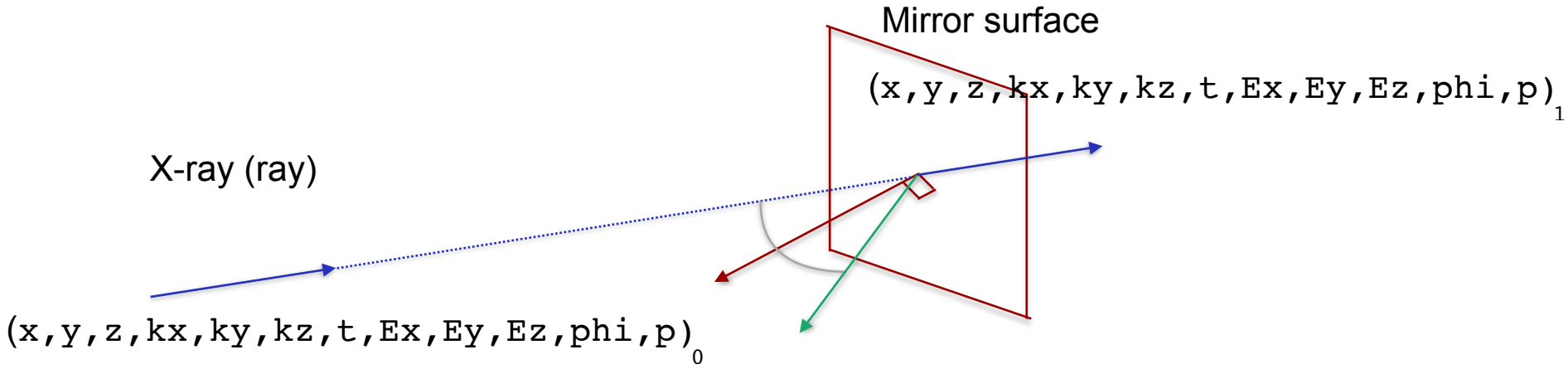
X-ray / matter interaction 1: reflecting surface

- 3. Checks (are we on surface, what is probability of reflection etc.)



X-ray / matter interaction 1: reflecting surface

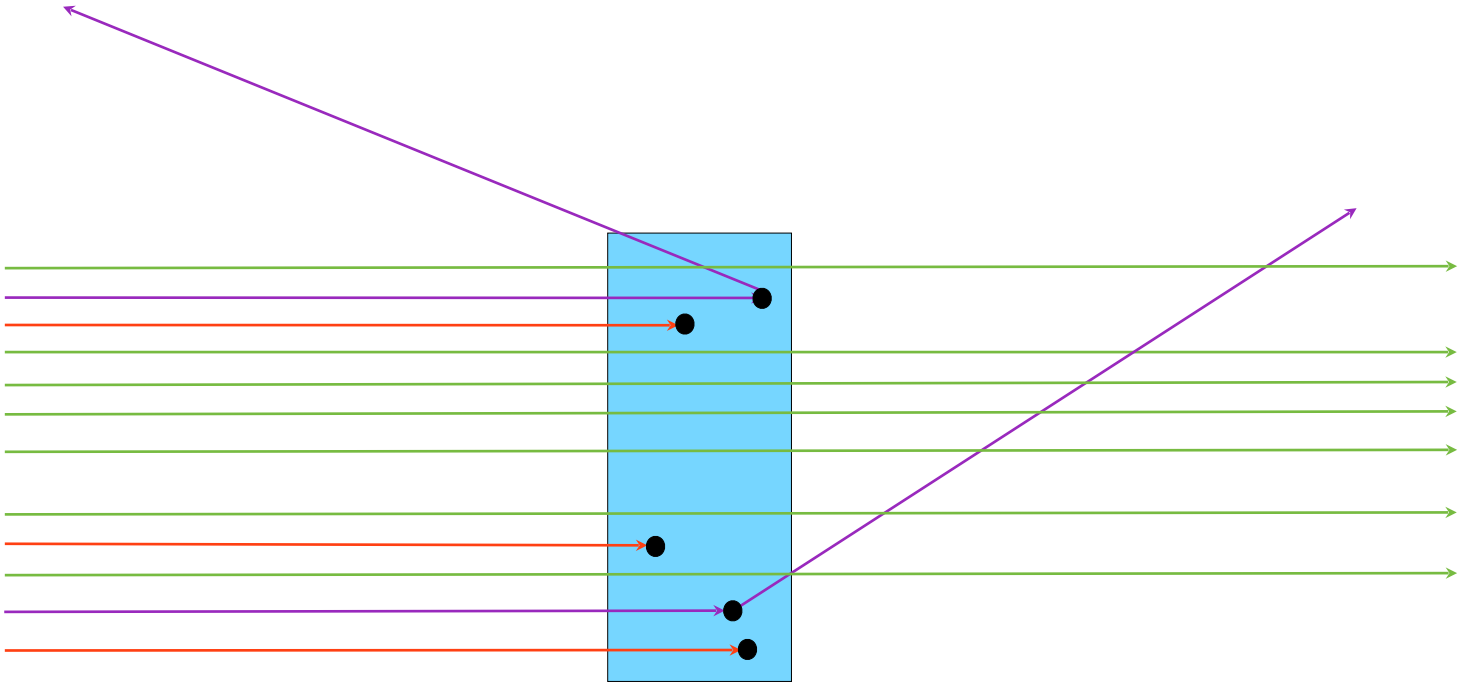
- 4. Reflect



Weight of final ray is adjusted according to reflectivity, see next slide

(x,y,z,kx,ky,kz,t,Ex,Ey,Ez,phi,p)2

X-ray / matter interaction in general



A photon hitting a sample can be:
absorbed, transmitted, or scattered

Samples

For a **non-thin** sample the probabilities for absorption, transmission or scattering are given by

$$p_A = (1 - e^{-\Sigma_T t})(\Sigma_A / \Sigma_T)$$

$$p_S = (1 - e^{-\Sigma_T t})(\Sigma_S / \Sigma_T)$$

$$p_T = 1 - p_S - p_A = e^{-\Sigma_T t}$$

t = sample thickness

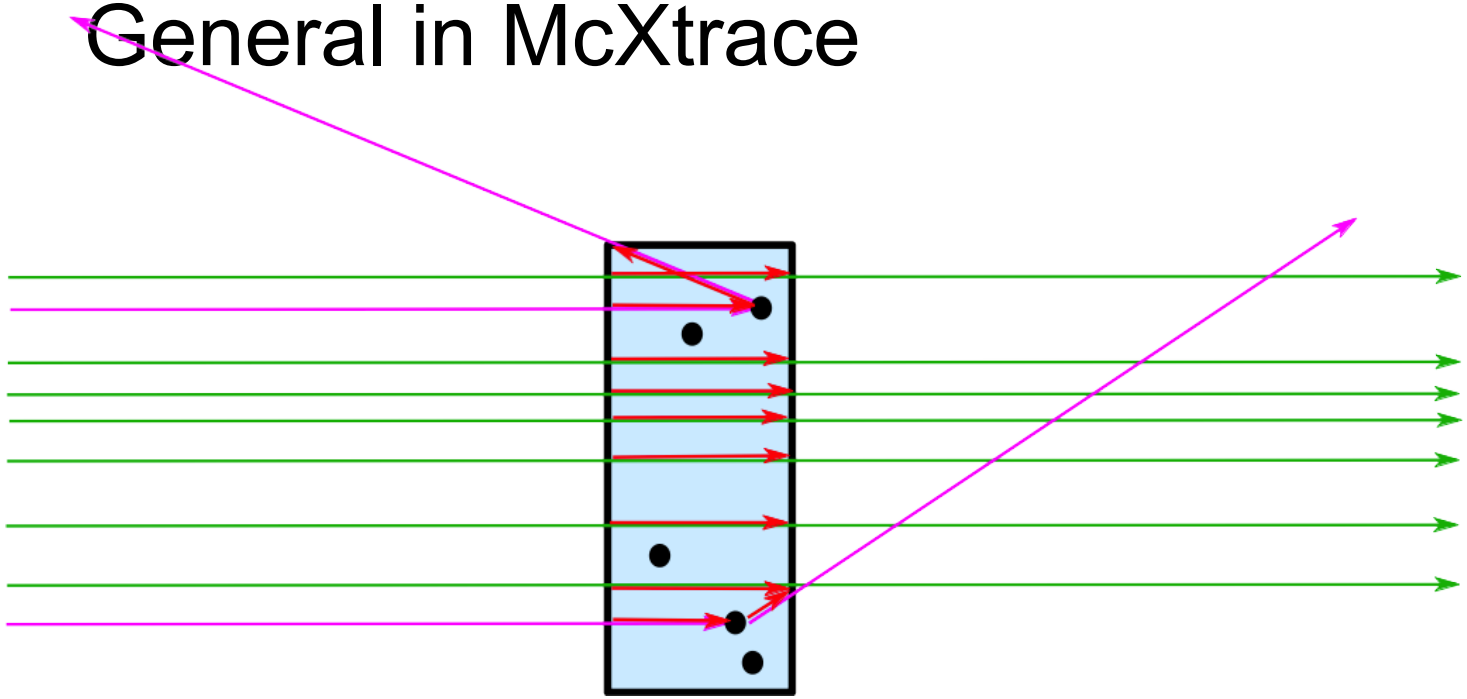
$$\Sigma_* = \rho \sigma_*$$

macroscopic cross section [cm^{-1}]

number density [$atoms/cm^3$]

microscopic cross section [$barn/fm^2$]

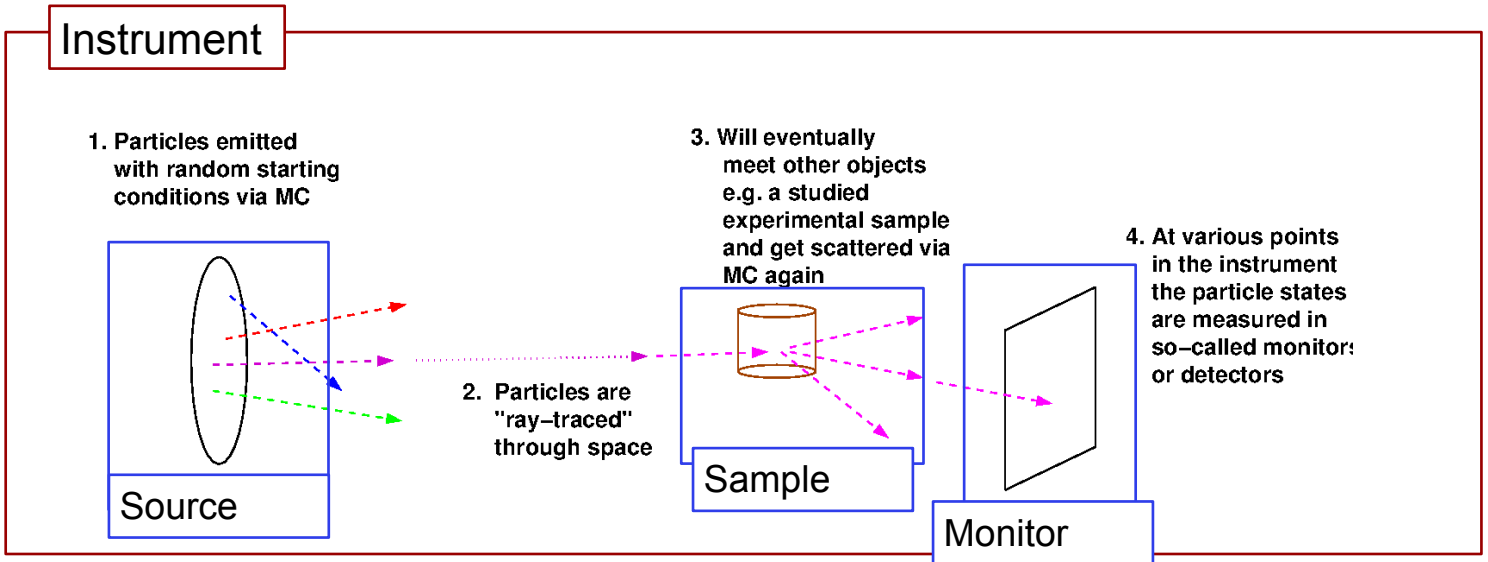
Samples/Matter interaction in General in McXtrace



A photon ray hitting a sample can be:
transmitted+absorption, or scattered+absorption

Transport of weight through the instrument…

In a given component, the X-ray intensity is adjusted by a multiplicative factor (probability)



p_0 p_j p_n

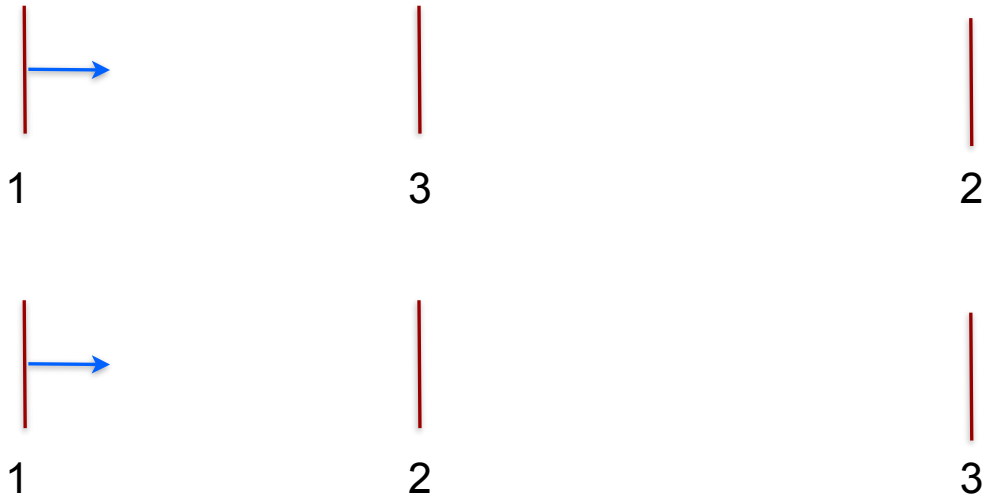
$$p_j = w_j p_{j-1}$$

The weight multiplier of the j'th component, w_j, is calculated by the probability rule $f_{\mathrm{MC,b}} w_j = P_{\mathrm{b}}$ where Pb is the physical probability for the event "b", and $f_{MC,b}$ is the probability that the Monte Carlo simulation selects this event.

In case of "branching", i.e. multiple outcomes, it is clear that $\sum_b f_{\mathrm{MC,b}} = 1$

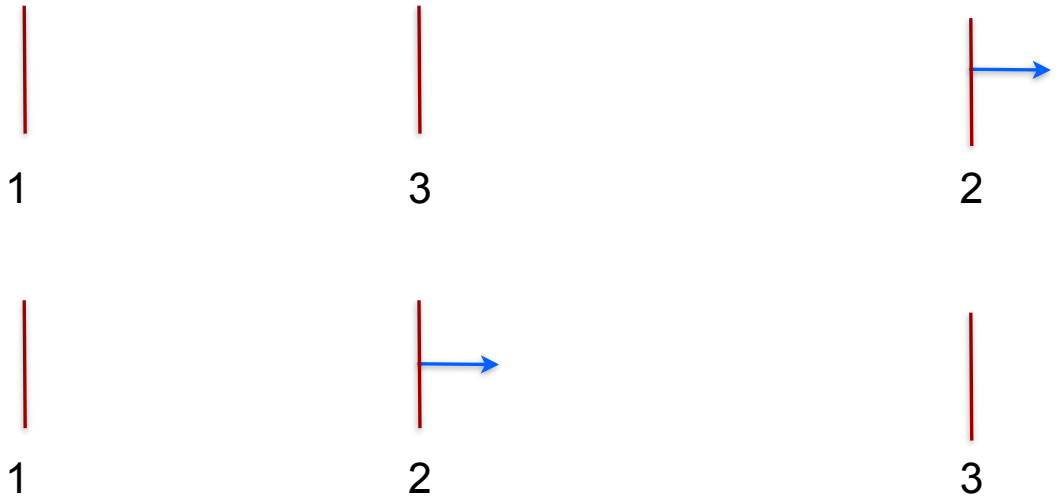
$$p_j = p_0 \prod_{k=1}^{j} w_k$$

To first order, McXtrace is linear and follows sequence of components in your file…



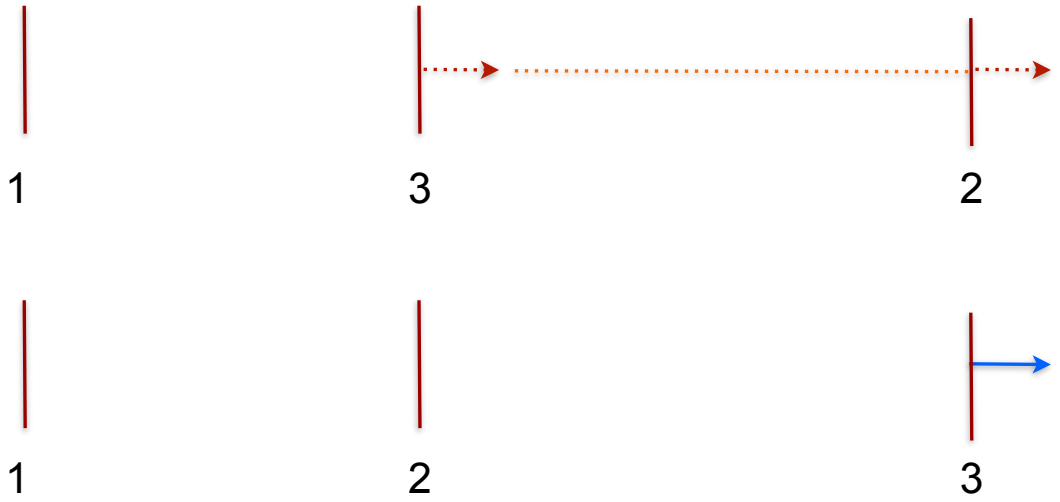
Starting at the source

To first order, McXtrace is linear and follows sequence of components in your file…



Moving to first comp in the list

To first order, McXtrace is linear and follows sequence of components in your file…



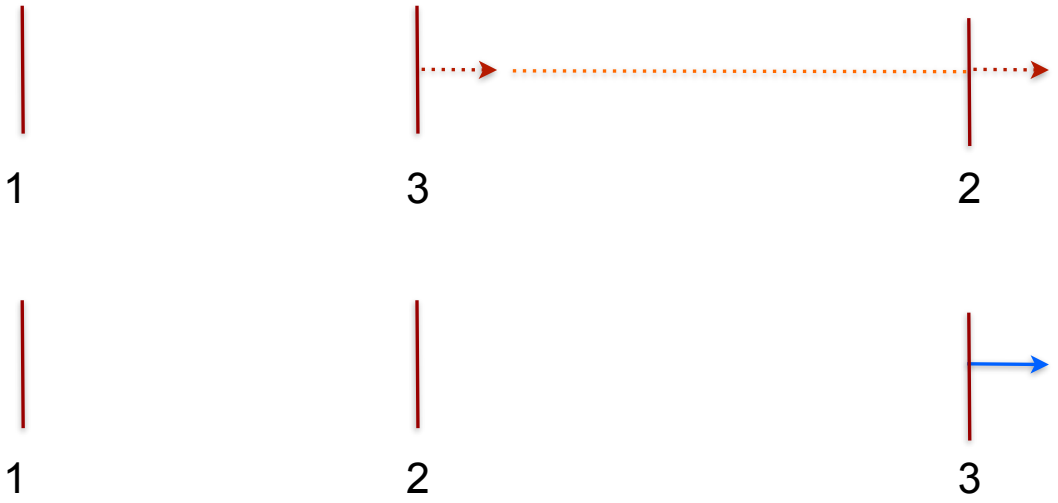
Moving to 3rd comp in list requires “moving back in time”.

Default behavior is to ABSORB this type of X-ray.

For monitors use restore_xray=1 in this case.

For homegrown comps use ALLOW_BACKPROP macro.

To first order, McXtrace is linear and follows sequence of components in your file…



Moving to 3rd comp in list requires “moving back in time”.

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The order of components is important,

and in general overlaps should be avoided!

Monitors: in general

REALITY:

Monitors:

- Intensity probe of the beam
- Semi-transparent to X-rays → Low Efficiency

Detectors:

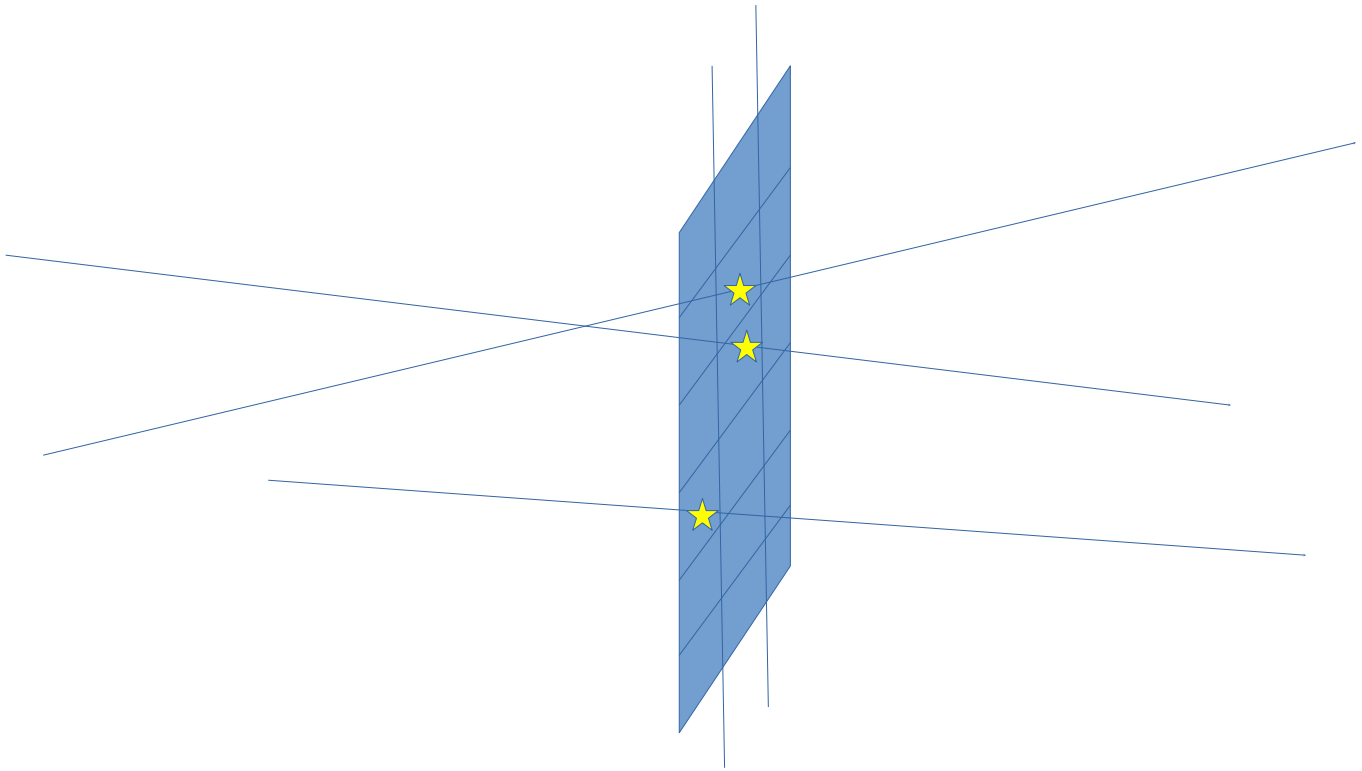
- Should detect *all* photons → Efficiency as high as possible

SIMULATIONS (McXtrace):

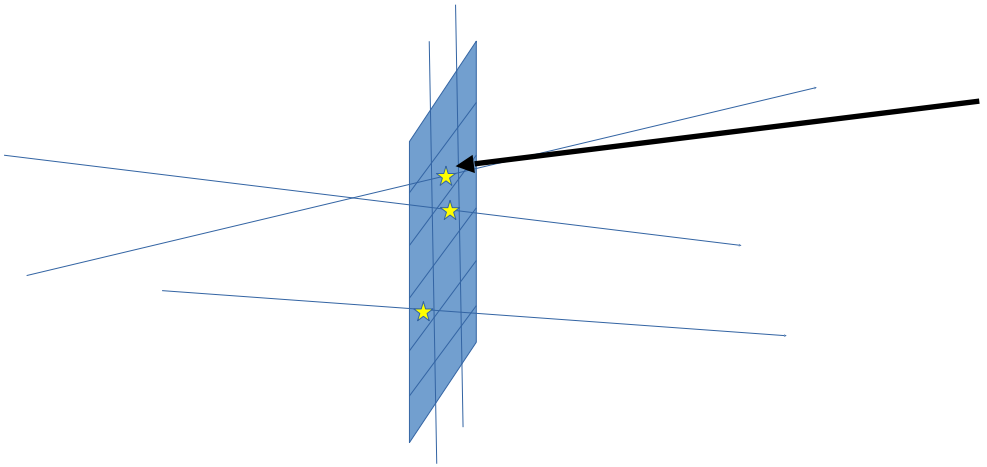
In McXtrace:

- We can program monitors and detectors to behave any way we like. We refer to both of those indistinguishably as ‘monitors’.
- E.g. monitor with Efficiency =100% and Transparency=100%

Monitors: Example PSD_monitor



Monitors: Example PSD_monitor

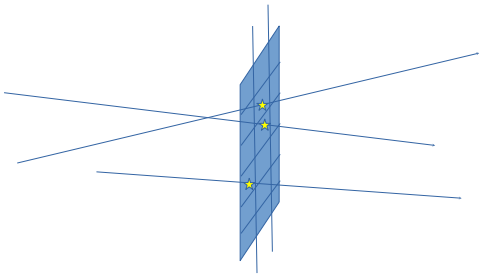


When the simulation has been completed, the detected intensity in pixel (i,j) is:

$$I(i,j) = \sum_{x_k,y_k \in pixel(i,j)} p_k; k = raynumber\,.$$

… during simulation, the pixels are maintained as running sums.

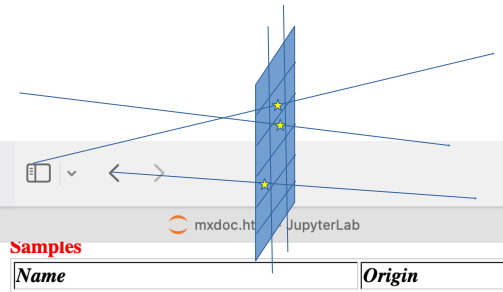
Monitors:
Example PSD_monitor and L_monitor

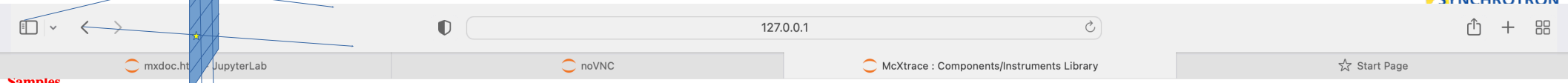


```
...
TRACE

COMPONENT origin = Progress_bar()
AT(0,0,0) ABSOLUTE


COMPONENT src = Source_flat(
          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


COMPONENT psd = PSD_monitor(xwidth=0.2,
          yheight=0.2, filename="psd.dat")
AT (0,0,5) RELATIVE src


COMPONENT lm = L_monitor(xwidth=0.2, yheight=0.2,
          filename="lm.dat",
          Lmin=0, Lmax=8)
AT (0,0,5+0.01) RELATIVE src
```

Monitors: what is available

mxdoc monitor from commandline





Samples

Name	*Origin*	*Author(s)*	*Source code*	*Description*

Detectors and monitors

Name	*Origin*	*Author(s)*	*Source code*	*Description*
PreMonitor_nD	ILL (France)	Emmanuel Farhi	comp	Release: McXtrace 1.1 Xray parameters spatial cross-correlation monitor.
PSD_monitor_coh	Risoe	Erik Knudsen	comp	Release: McXtrace 0.1 Position-sensitive monitor with phase intergration.
E_monitor	Risoe	Erik Knudsen	comp	Release: McXtrace 0.1 Energy-sensitive monitor.
L_monitor	Risoe	Kristian Nielsen and Kim Lefmann	comp	Release: McXtrace 0.1 Wavelength-sensitive monitor.
Divergence_monitor	DTU Physics	Erik B Knudsen	comp	Horizontal+vertical divergence monitor.
TOF_monitor	British Airways	Erik B Knudsen	comp	Release: 1.2 Rectangular Time-of-flight monitor. %P INPUT PARAMETERS: xmin: Lower x bound of detector opening (m) xmax: Upper x bound of detector opening (m) ymin: Lower y bound of detector opening (m) ymax: Upper y bound of detector opening (m) xwidth: Width of detector. Overrides xmin,xmax. (m) yheight: Height of detector. Overrides ymin,ymax. (m) nt: Number of time bins (1) dt: Length of each time bin (mu-s) tmin: Lower time limit (mu-s) tmax: Upper time limit (mu-s) filename: Name of file in which to store the detector image (text) restore_xray: If set, the monitor does not influence the xray state (1) OUTPUT PARAMETERS: TOF_N: Array of xray counts TOF_p: Array of xray weight counts TOF_p2: Array of second moments
EPSD_monitor		Erik B Knudsen	comp	
Monitor	Risoe	Erik Knudsen	comp	Release: McXtrace 0.1 Energy-sensitive monitor.
DivPos_monitor	DTU Physics	Erik B Knudsen	comp	Release: McXtrace 1.3 Divergence/position monitor (acceptance diagram).
PSD_monitor	Risoe	Erik B Knudsen	comp	Position-sensitive monitor.
Monitor_nD	ILL	Emmanuel Farhi	comp	Release: McXtrace 1.6 This component is a general Monitor that can output 0/1/2D signals (Intensity or signal vs. [something] and vs. [something] ...)
PSD_monitor_4PI	Risoe	Erik Knudsen	comp	Release: McXtrace 0.1 Spherical position-sensitive detector.
W_psd_monitor	Risoe	Erik Knudsen	comp	Release: McXtrace 0.1 Position-sensitive wattage monitor.
DivE_monitor	DTU Physics	Erik B Knudsen	comp	Divergence/Energy monitor.

Misc

Name	*Origin*	*Author(s)*	*Source code*	*Description*

Contributed components

Name	*Origin*	*Author(s)*	*Source code*	*Description*
SAXSQMonitor	KU-Science	Martin Cramer Pedersen (mcpe@nbi.dk)	comp	Release: McXtrace 1.0 A circular detector measuring the radial average of intensity as a function of the momentum transform in the sample.

Obsolete (avoid usage whenever possible)

Name	*Origin*	*Author(s)*	*Source code*	*Description*

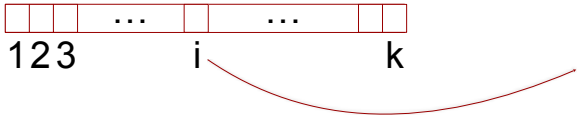
Instrument Examples

Name	*Origin*	*Author(s)*	*Source code*	*Description*
Focal_pt_monitor	DTU Physics	Erik B Knudsen (erkn@fysik.dtu.dk)	instr	Template for creating a focal point monitor.
Test_monitors	DTU Physics	Erik B Knudsen (erkn@fysik.dtu.dk)	instr	Unit test instrument for various monitors.

Local components

In a histogram sense

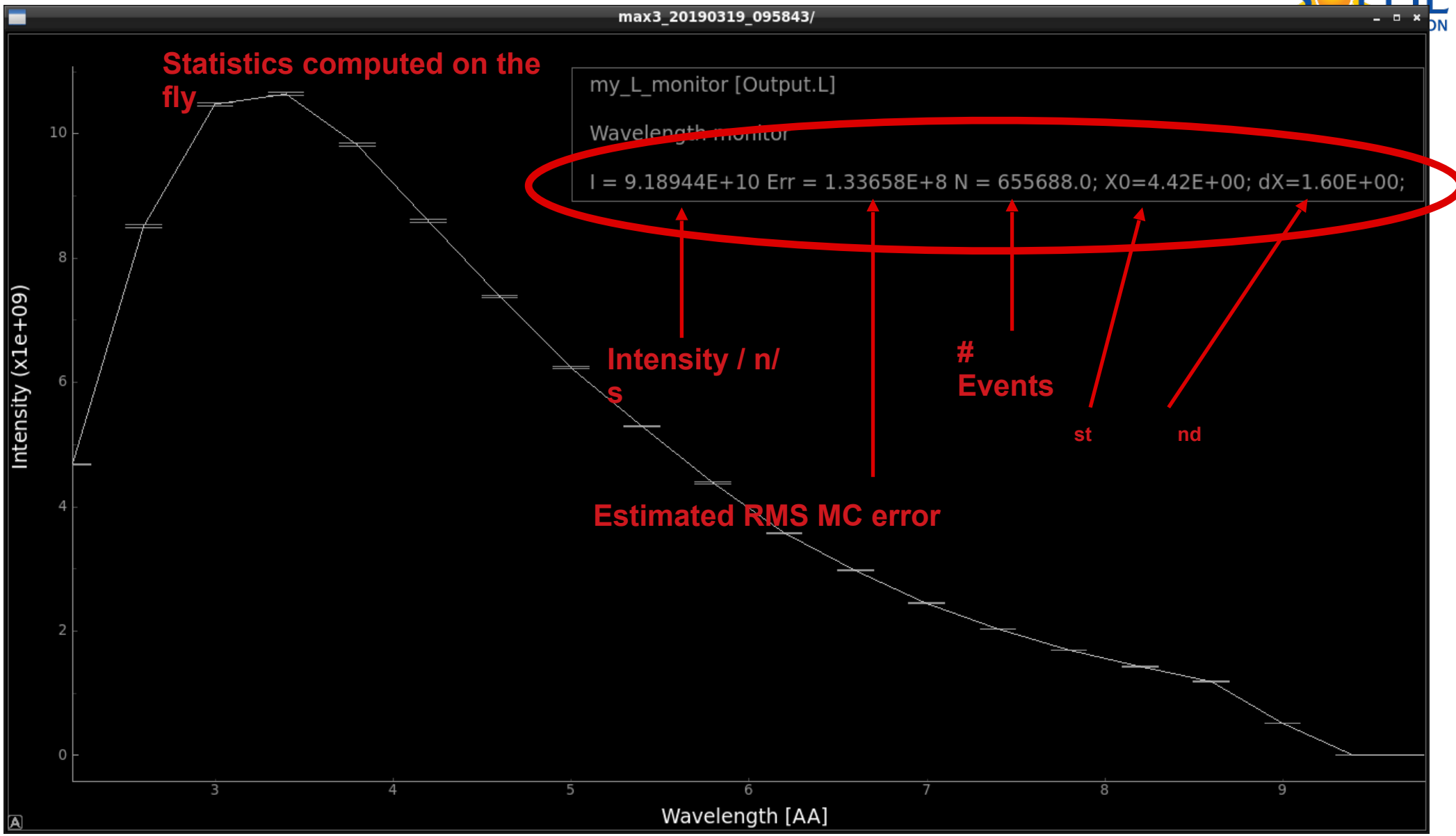
- Imagine a histogram, e.g. **I**(λ)

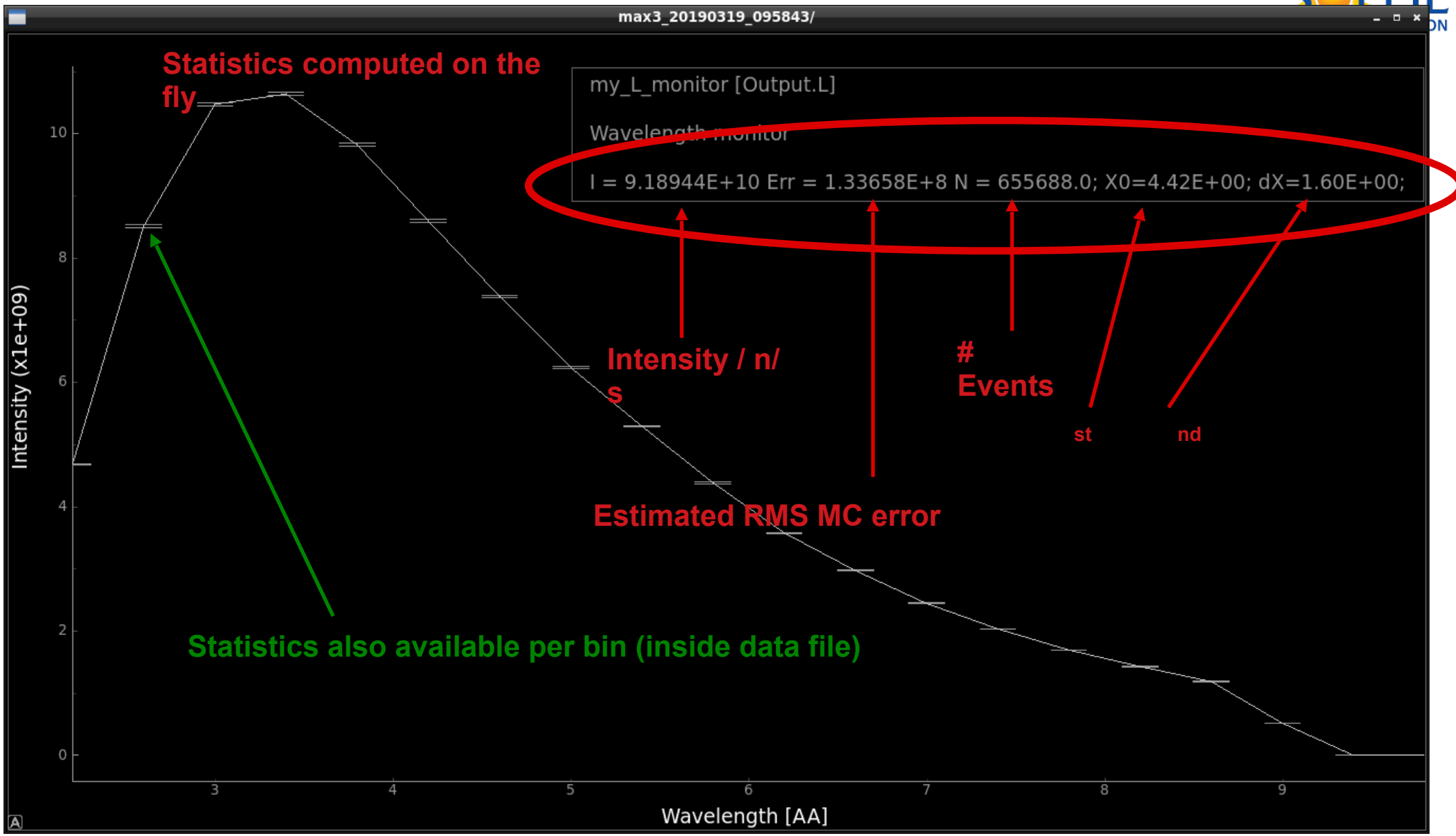


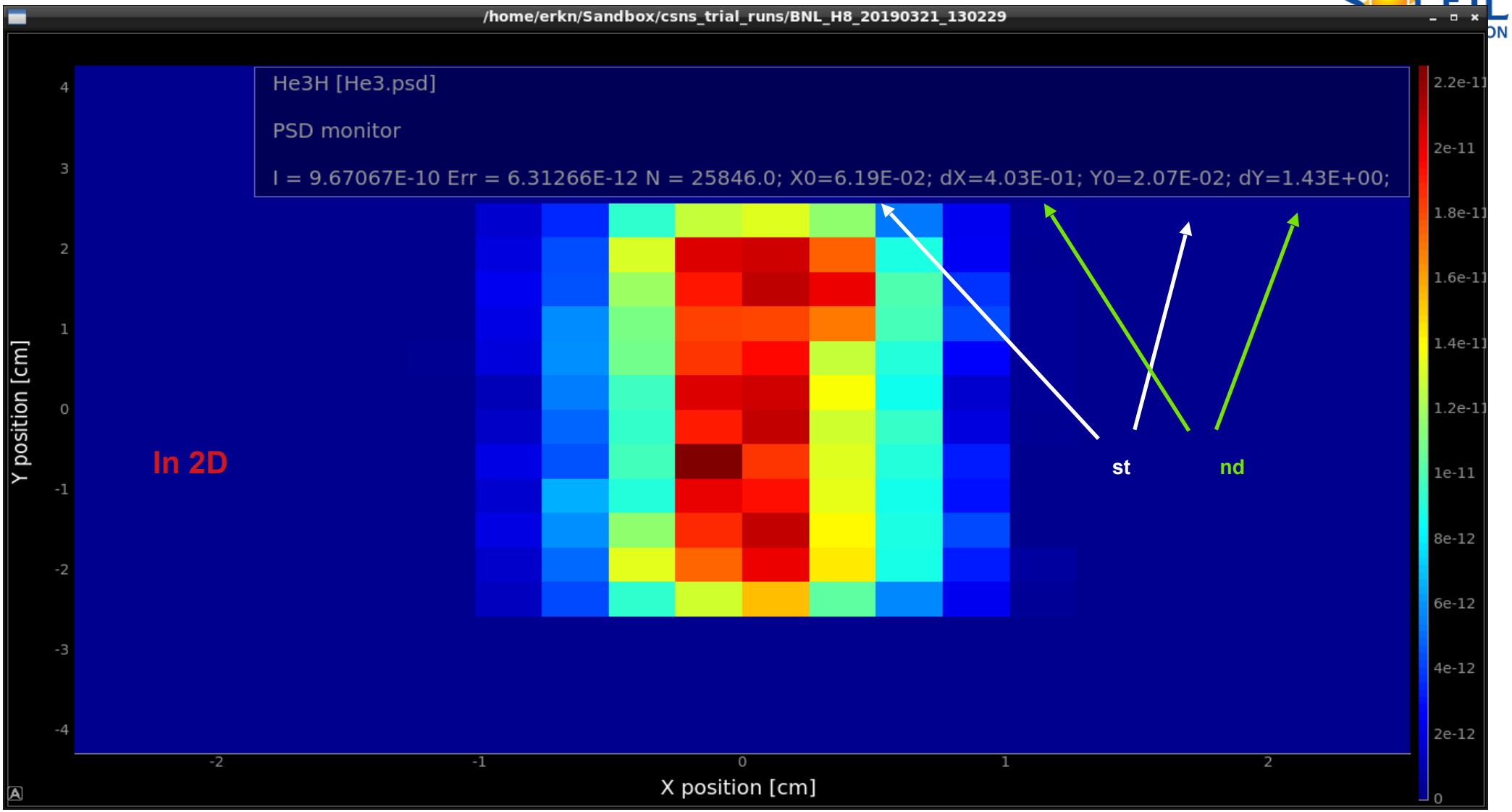
$$I = \sum_{N} p_j$$

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

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


max3_20190319_095843/
Statistics computed on the fly
my_L_monitor [Output.L]
Wavelength monitor
I = 9.18944E+10 Err = 1.33658E+8 N = 655688.0; X0=4.42E+00; dX=1.60E+00;
Intensity / n/ s
Events
st
nd
Estimated RMS MC error
Intensity (x1e+09)
Wavelength [AA]
0
2
4
6
8
10
3
4
5
6
7
8
9


max3_20190319_095843/
Statistics computed on the fly
my_L_monitor [Output.L]
Wavelength monitor
I = 9.18944E+10 Err = 1.33658E+8 N = 655688.0; X0=4.42E+00; dX=1.60E+00;
Intensity / n/ s
Events
st
nd
Estimated RMS MC error
Statistics also available per bin (inside data file)
Intensity (x1e+09)
Wavelength [AA]
0
2
4
6
8
10
3
4
5
6
7
8
9


/home/erkn/Sandbox/csns_trial_runs/BNL_H8_20190321_130229
He3H [He3.psd]
PSD monitor
I = 9.67067E-10 Err = 6.31266E-12 N = 25846.0; X0=6.19E-02; dX=4.03E-01; Y0=2.07E-02; dY=1.43E+00;
In 2D
st
nd
Y position [cm]
X position [cm]
4
3
2
1
0
-1
-2
-3
-4
-2
-1
0
1
2
2.2e-11
2e-11
1.8e-11
1.6e-11
1.4e-11
1.2e-11
1e-11
8e-12
6e-12
4e-12
2e-12
0

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

$$I = \sum_{i=1}^{n} w_i. \tag{1}$$

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

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

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

$$C = tI, \tag{3}$$

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

$$\sigma^2(C) = t^2\sigma^2(I). \tag{4}$$

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

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

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

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

The standard deviation for the VE becomes

$$\sigma^2_{\mathrm{VE}}(C) = t^2\sigma^2(I) + \Sigma^2. \tag{7}$$

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

$$\Sigma^2 = tI - t^2\sigma^2(I). \tag{8}$$

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

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

Sketch of an algorithm…

1. On a given McXtrace 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…

DTU

McXtrace

SOLEIL SYNCHROTRON

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

Monitor_nD

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

***Monitor_nD** can have almost any shape, and record*

any requested standard quantities

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

Monitor_nD

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

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

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")
```