McStas data normalisation

- *and other important, not so well known details*

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Topics

- From the McStas FAQ's:
  - Why comps in this order?
  - Simulation to experiment comparison (Data normalisation)
  - How to make your McStas more efficient
  - Other important details

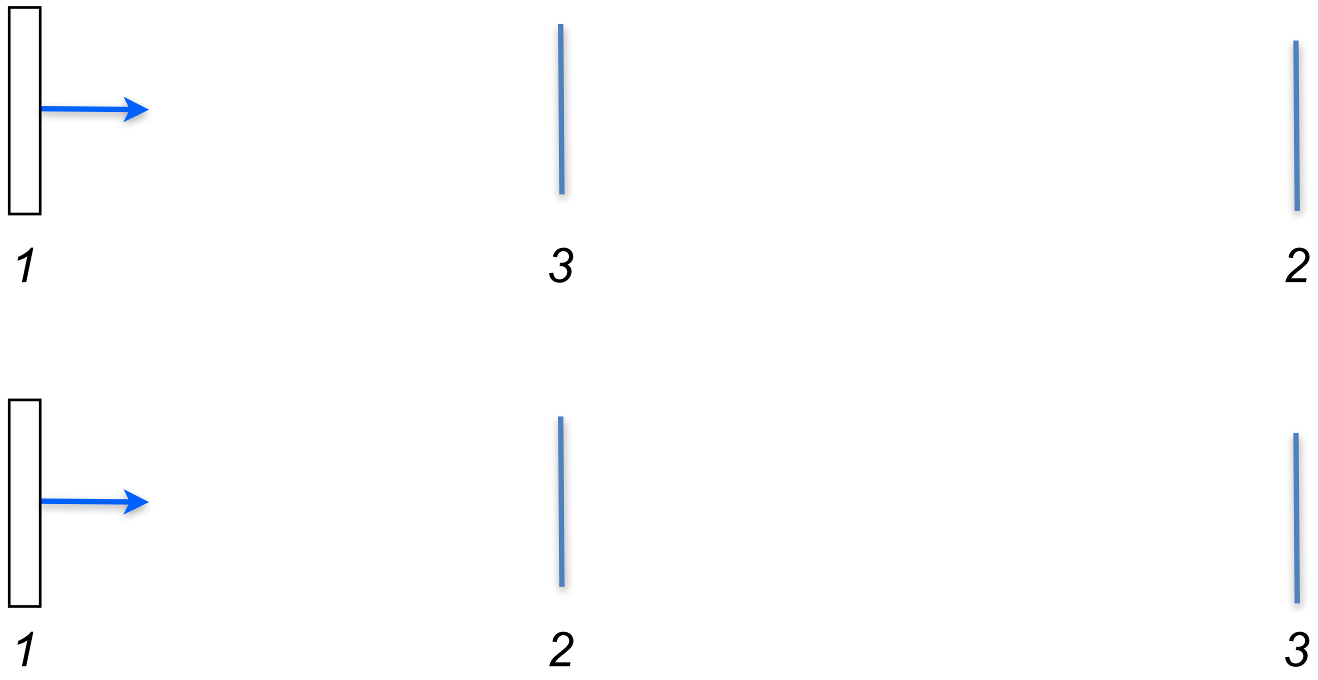
From the “list of frequent questions”

October 2018

- *Why do you need to have the components in this order?*

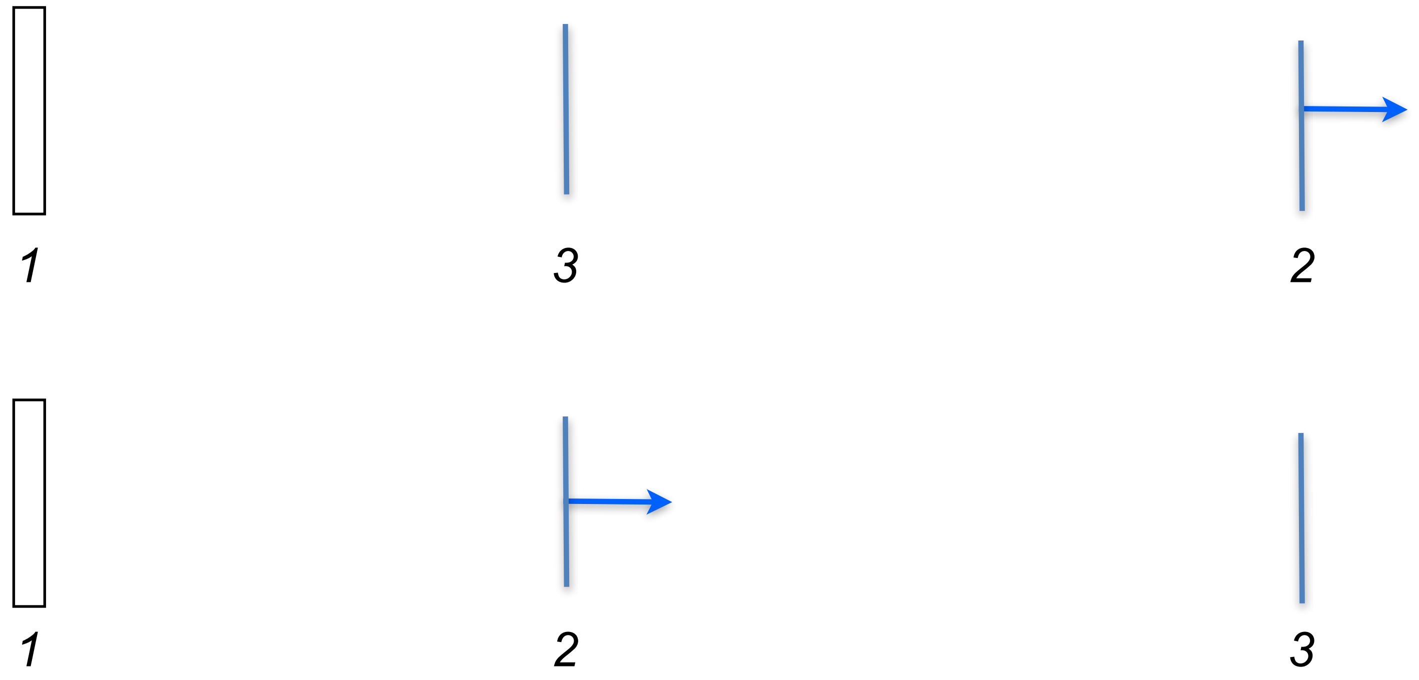
Order of components is important

October 2018



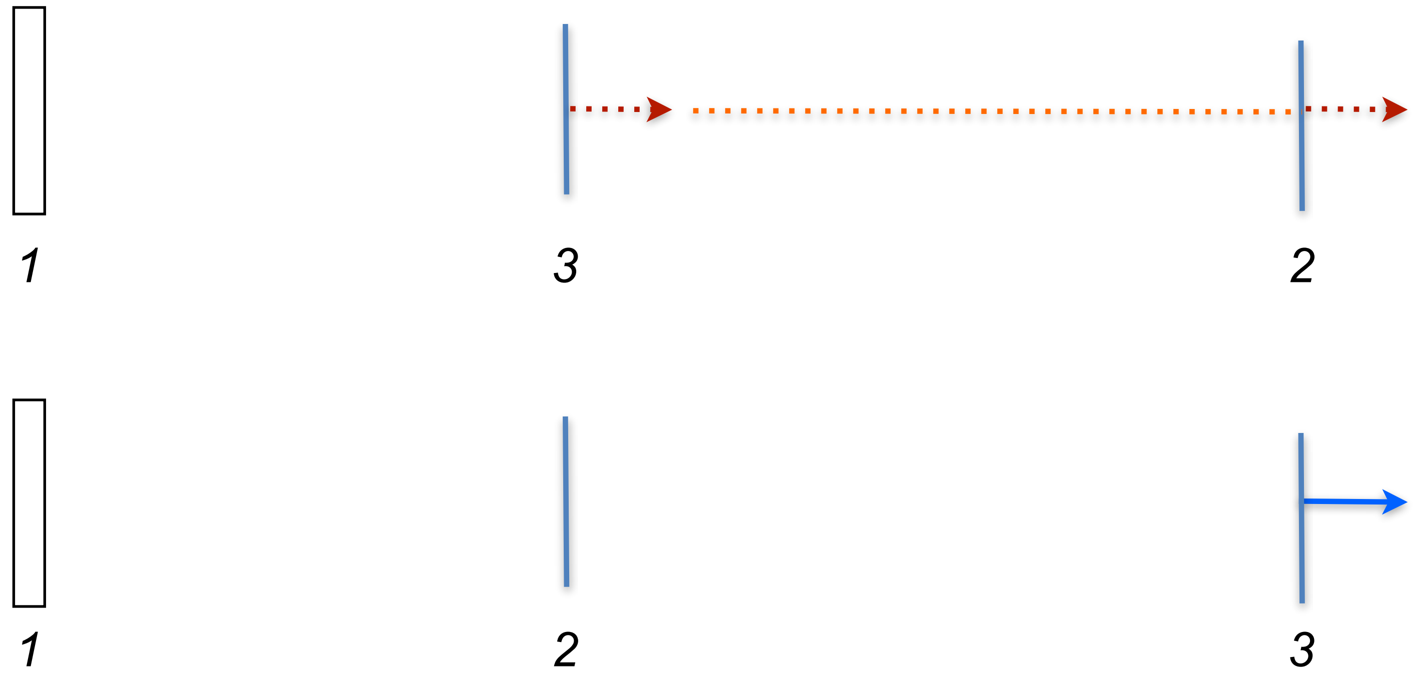
Starting at the source

Order of components is important



Moving to first comp in the list

Order of components is important



Moving to 3rd comp in list requires "moving back in time".
Default behavior is to ABSORB this type of neutron.
For monitors use restore_neutron=1 in this case.
For homegrown comps use ALLOW_BACKPROP macro.

Further tips 1:

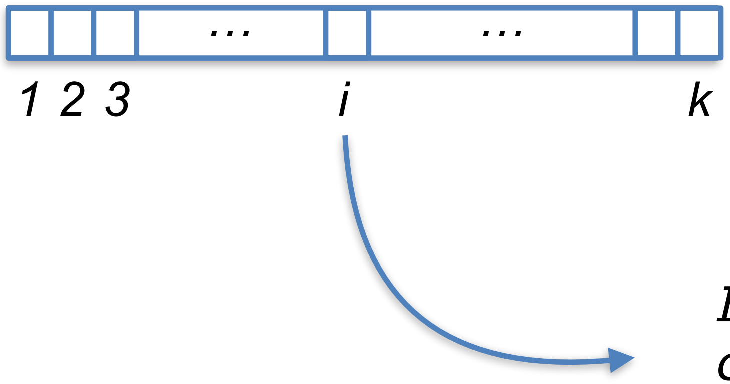
- Simulation to experiment comparison
-

What is really the information content…?

- McStas sources generally provide "intensity" in units of neutrons/s (into a chosen solid angle)
- That intensity is carried through the instrument on a discrete set of "neutron rays"

In a histogram sense

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



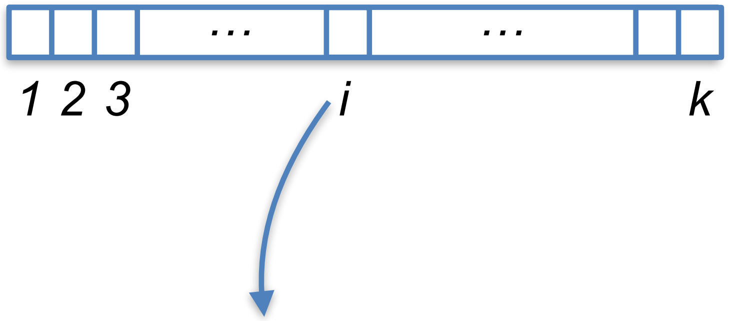
In bin i, N events each carrying a fractional intensity p_j so that

$$I = \sum_N p_j$$

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

In a histogram

- *Imagine a histog*



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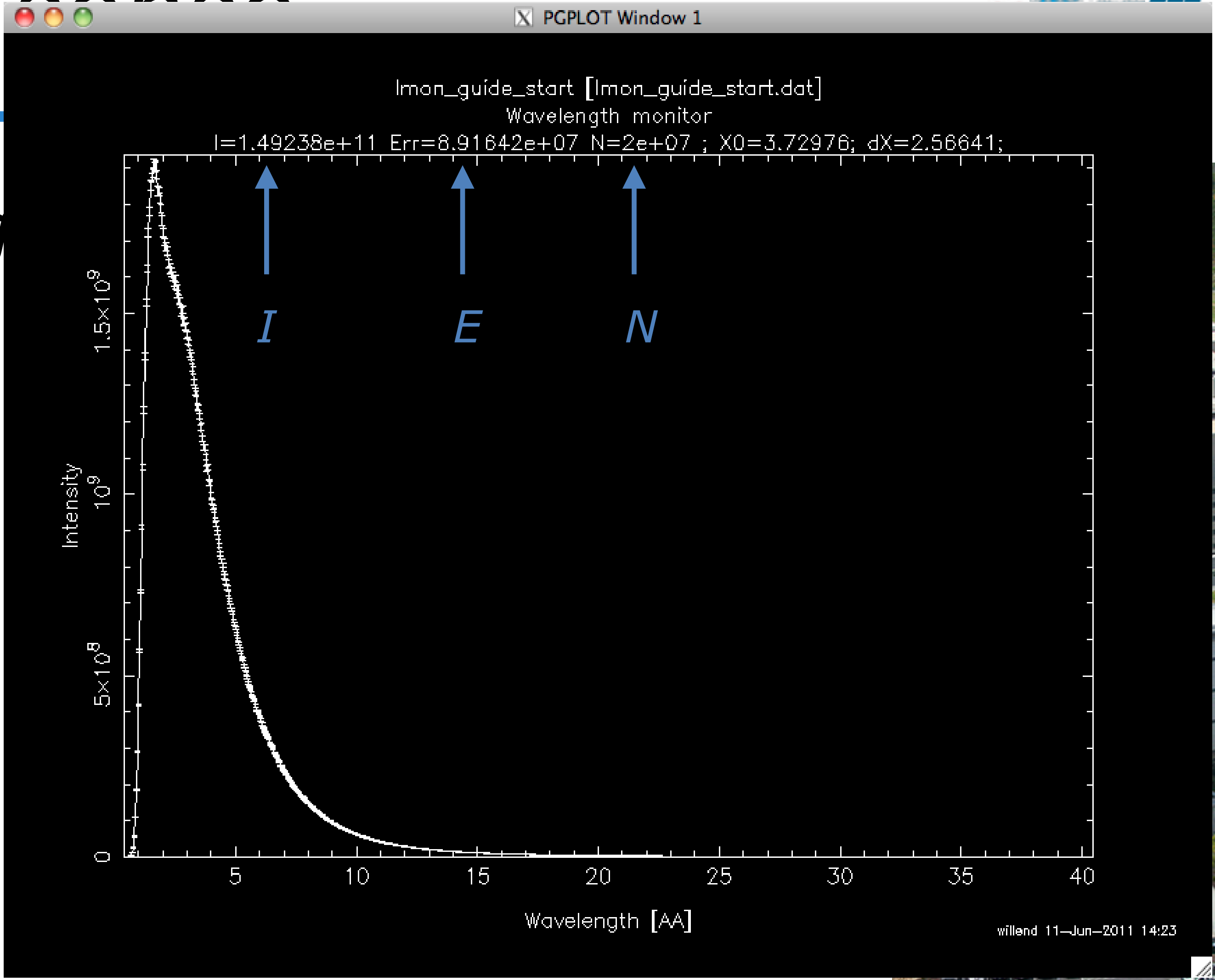

- *The RMS variance over that set becomes our statistical error bar E*

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

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

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

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

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

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

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

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

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

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

The standard deviation for the VE becomes

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

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

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

Sketch of an algorithm…

1. On a given McStas histogram

2. For the non-zero bins, calculate

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

3. The smallest $t_{\mathtt{max}}$ defines the "maximal counting time" allowed by your statistics

4. Preferably a "background" should be added - use a "known experimental value" or an estimate…

Important points to remember

1. Your simulation will only contain elements you provided / defined

2. … to the precision you defined

3. Answers the questions you posed

4. Background essentially only from "sample", or sample-near objects

Further tips 2:

- How to make your McStas more efficient

Onto efficiency…

- ✦*Apply focusing techniques*
  - ✦*At the source (spatially, temporally, in wavelength…)*
  - ✦*At the sample, if possible*
- ✦*(carefully!) Apply SPLIT - but only if immediately followed by Monte Carlo choices, e.g. in sample*
- ✦*Alternatively use MCPL o/i which allows repetition - beware of biases!*

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All of this can be considered "variance reduction" or biasing

Onto efficiency…

- ✦Use MPI parallelisation - included in macOS install from 2.4.1, easy to get on Linux… On Windows McStas uses MS MPI, get it from "extras" folder where you downloaded 2.4.1
- ✦The Intel C compiler is known to give ~factor of 2 wrt. gcc in most cases
- ✦- Still consider if you are asking the right question if runtimes reach days/weeks…

Sledge-hammer / brute force!