

Reverse tracing in SIMRES & McStas

Towards faster ray-tracing simulations

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Variance reduction in MC ray-tracing

Ray-tracing employs the *rejection sampling* method, which suffers from very low event probability, p ... becomes worse with increasing dimension

Relative variance for binomial distribution:
$$\frac{\sigma}{p} = \sqrt{\frac{1-p}{Np}}$$

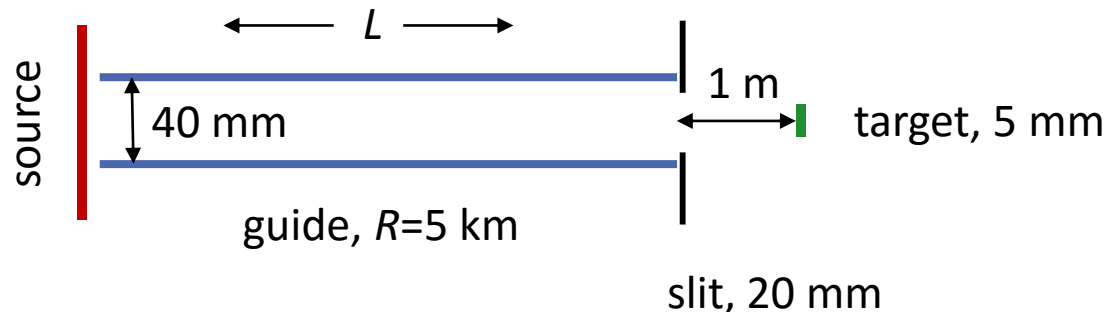
p can be increased by optimization of the sampling volume
(typically n -dimensional box, $n \geq 6$)

What is the optimum sampling volume ?

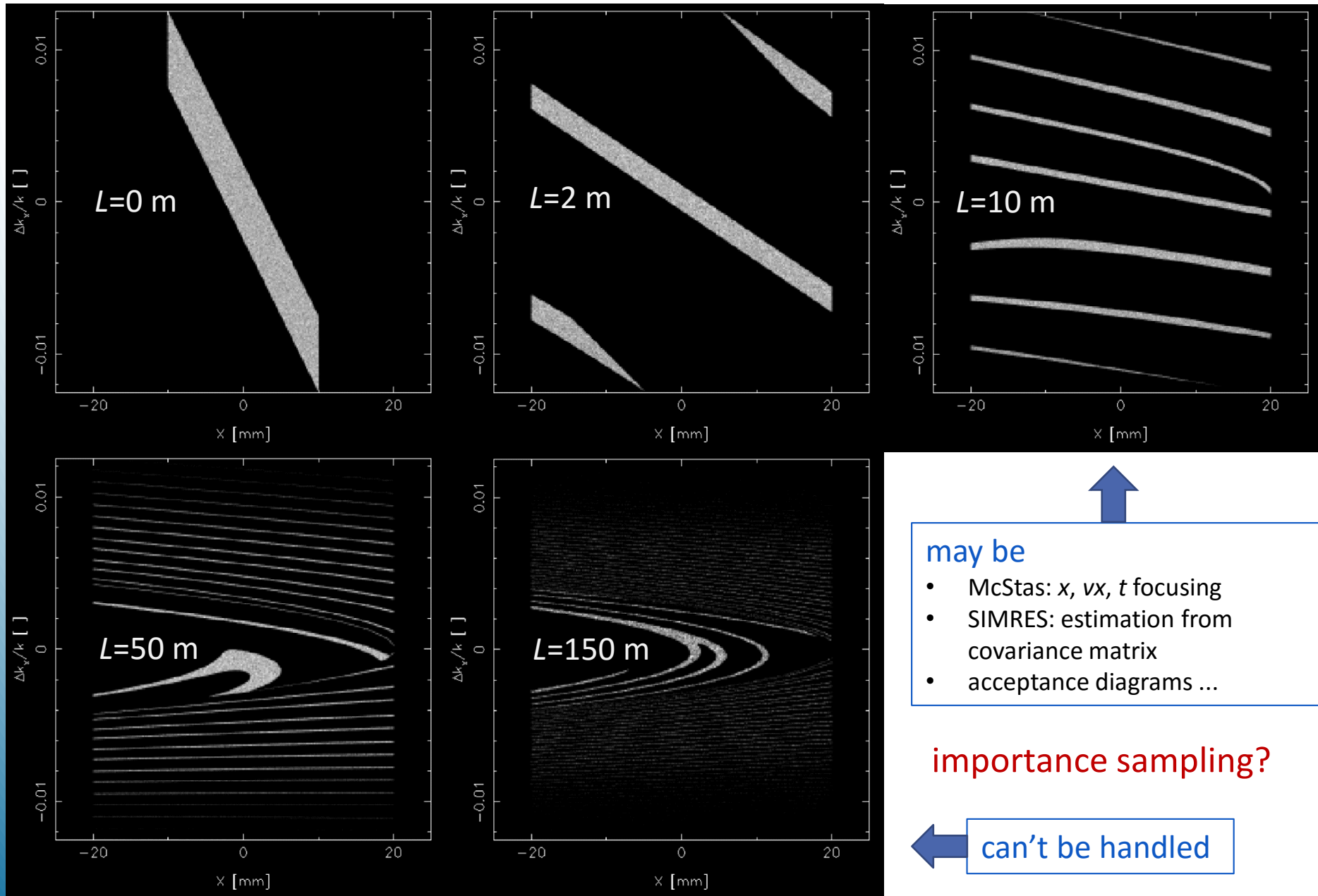
Consider simple 2-dimensional example:

Usual situation: sample << source

How to choose x, v_x at the source
to hit the sample?



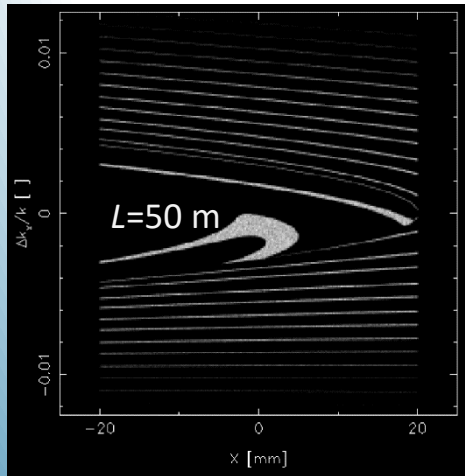
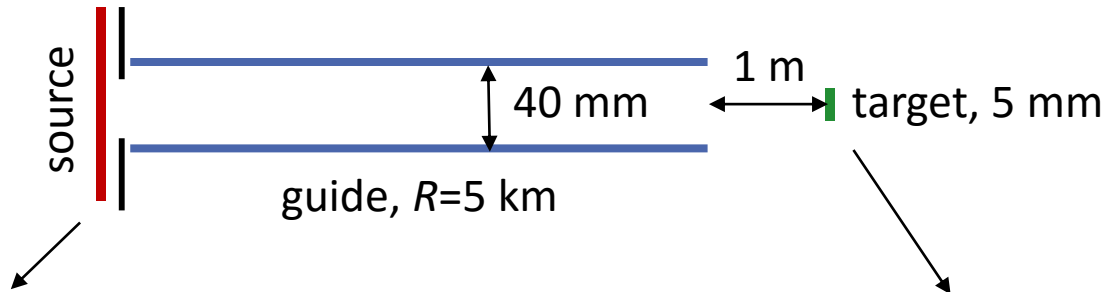
Optimum sampling volume as a function of guide length



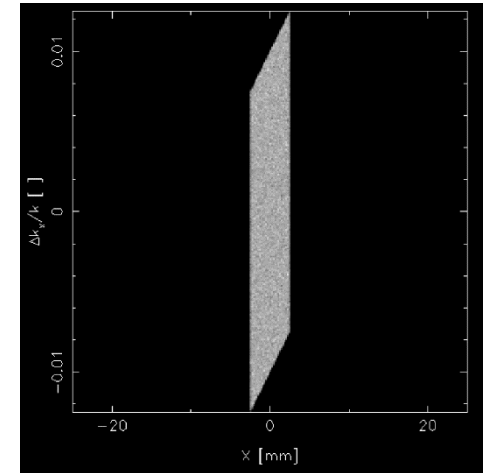
Reversibility of ray-tracing

Reversibility is guaranteed by the invariance of underlying physical laws with respect to time inversion:

$$\mathbf{p}' = -\mathbf{p} , \quad t' = -t$$



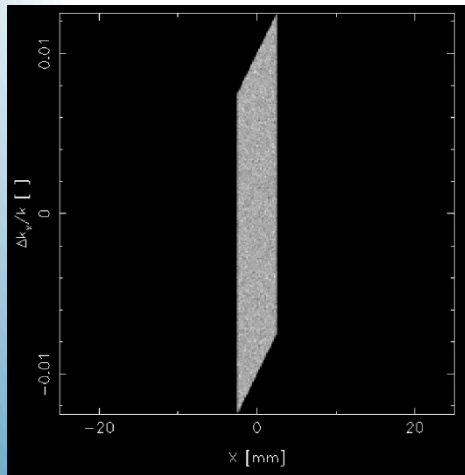
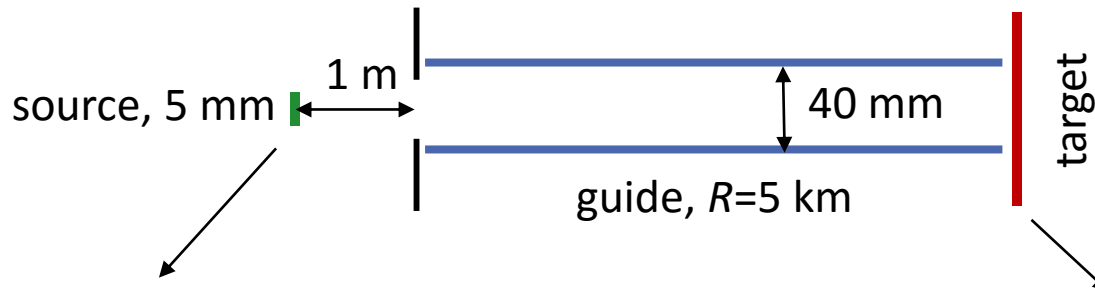
Isomorphism between the two spaces
= there is an inverse map ...



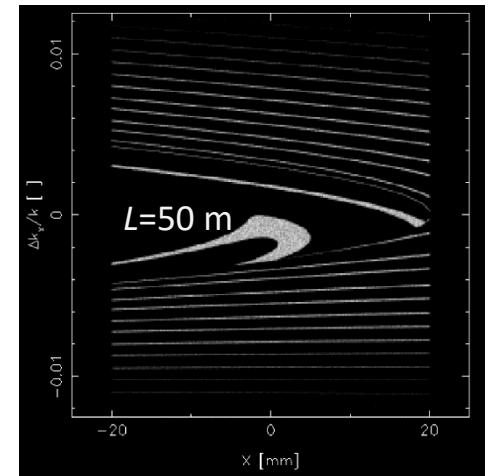
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Isomorphism between the two spaces
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Solutions

- allow tracing in any direction (SIMRES)
- or build an inverted instrument model (McStas)

Variance reduction by reverse ray-tracing

Prerequisites for true reverse tracing

- SW components must handle tracing in any direction
- ✗ Neutron generator must be decoupled from the moderator.
- ✗ Simulation kernel must handle the \mathbf{p} , t reversal.

Not implemented in McStas



the workaround solution requires

- instrument inversion
- two special components for tracing reversal
- modification of moderators

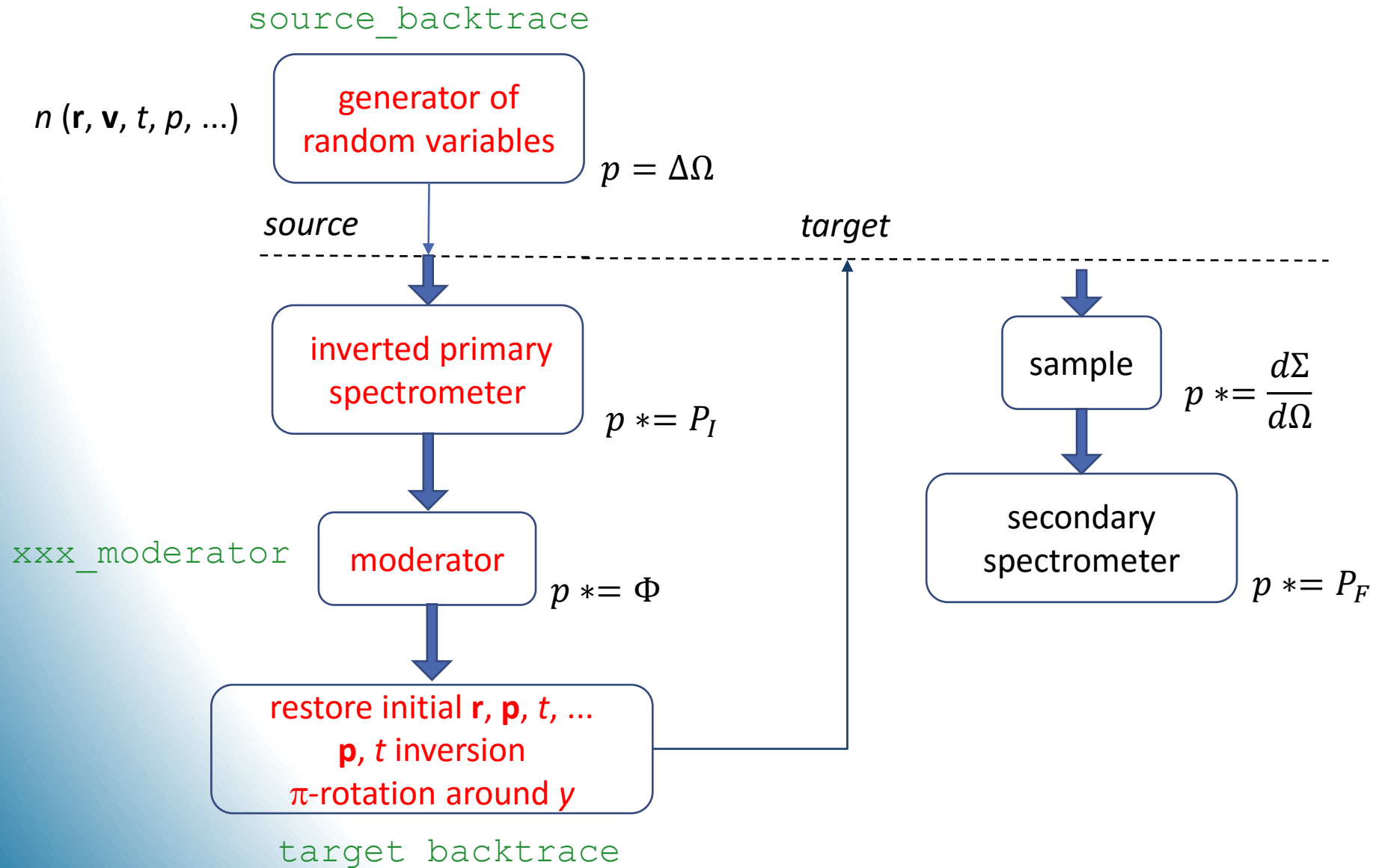
Work done in early 2016:

Simple example for McStas

- Includes required new components and instrument files for testing
- Can be used as a template for real work
- Presented at the last WP8 meeting

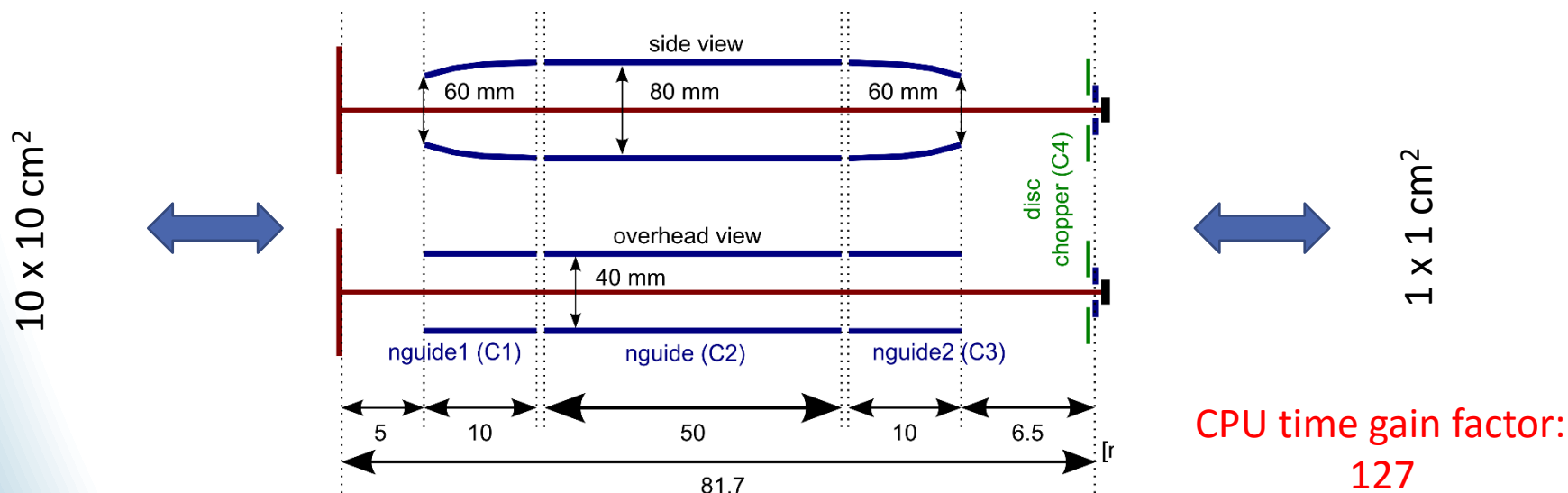
Reverse tracing in McStas

new McStas components

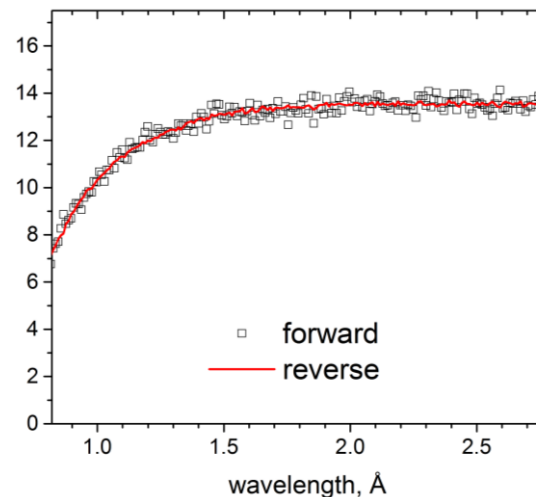
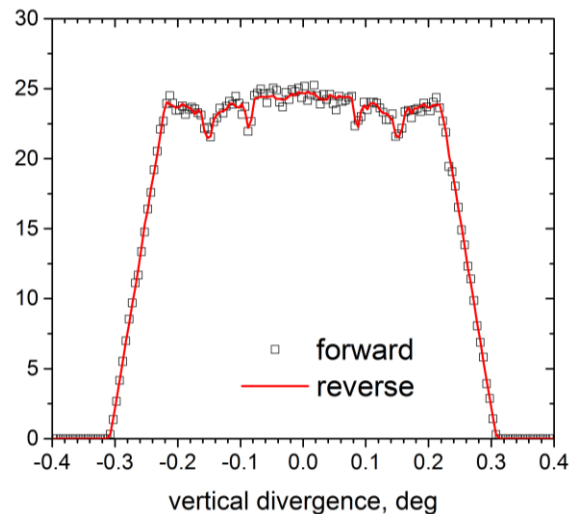
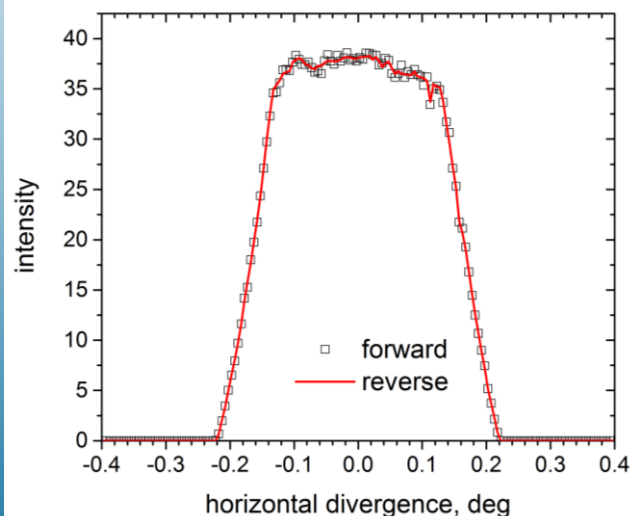


Simple instrument example

- includes commented source code
- short manual to be finished

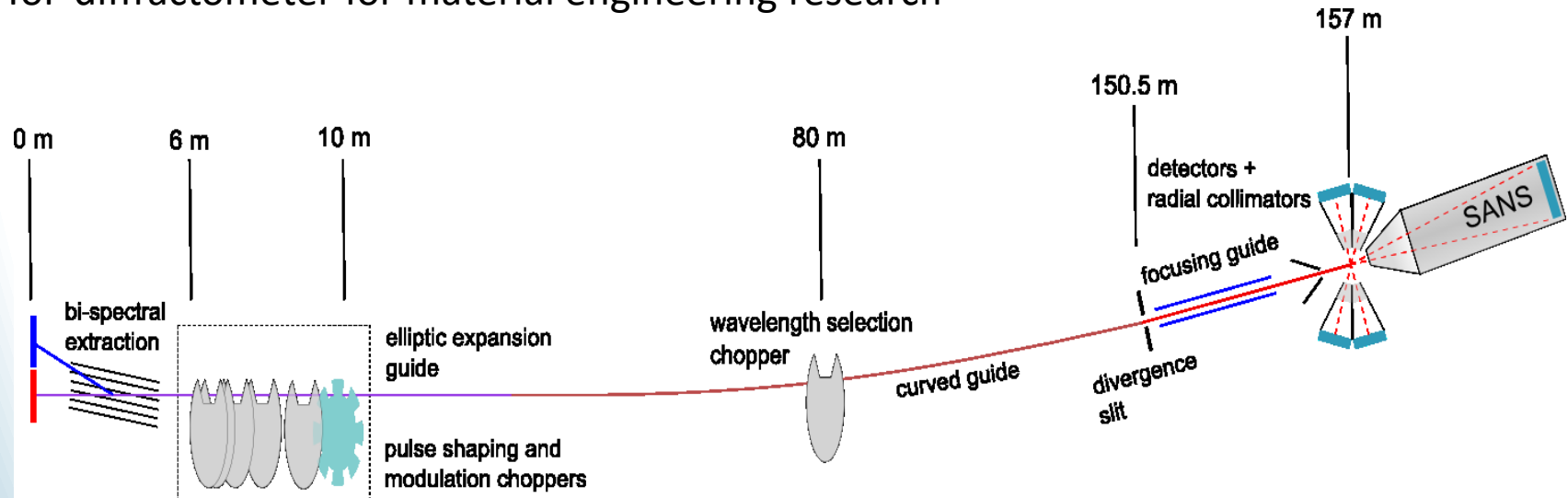


CPU time gain factor:
127



Application to BEER@ESS

ToF diffractometer for material engineering research



McStas model:

- includes 35 components
- primary spectrometer written in two versions: direct and inverted (both are defined by the same set of input parameters)
- 2 adapted components (ESS moderator and diffraction monitor)
- 1 new component (semi-transparent multichannel guide)

Application to BEER@ESS

Added code:

ESS_Moderator_backtrace.comp

plus `ess_source-lib-NPI` (extension to the McStas library)

Provides ESS moderator brightness functions without actually generating neutrons (just adding weights). *Only version 2014 (pancake) is done, implementation of the butterfly model is planned after the McStas update release.*

PSDcyl_dhkl_monitor.comp

Adapted `PSDcyl_monitor.comp`, generates diffractograms from detected neutron positions in 3D (x, y, t).

Runtime parameters for high-level instrument control:

```
DEFINE INSTRUMENT BEER(lam0 = 1.8, dlam = 1, frac = 1, int operating_mode = 6,  
Guide_curvature = 0.06,int verbose = 0, S1_width = 0.040, S1_height = 0.0684,  
S2_width = 0.040,S2_height = 0.0502, S3_width = 0.005, S3_height = 0.010, S3_dist  
= 0.050, int GF3a_on = 1)
```

TRACE

```
%include "input_parameters.instr"  
// choose tracing direction:  
//%include "BEERforward.instr"  
%include "BEERreverse.instr"  
%include "secondary_part.instr"
```

Other parameters are provided in a file

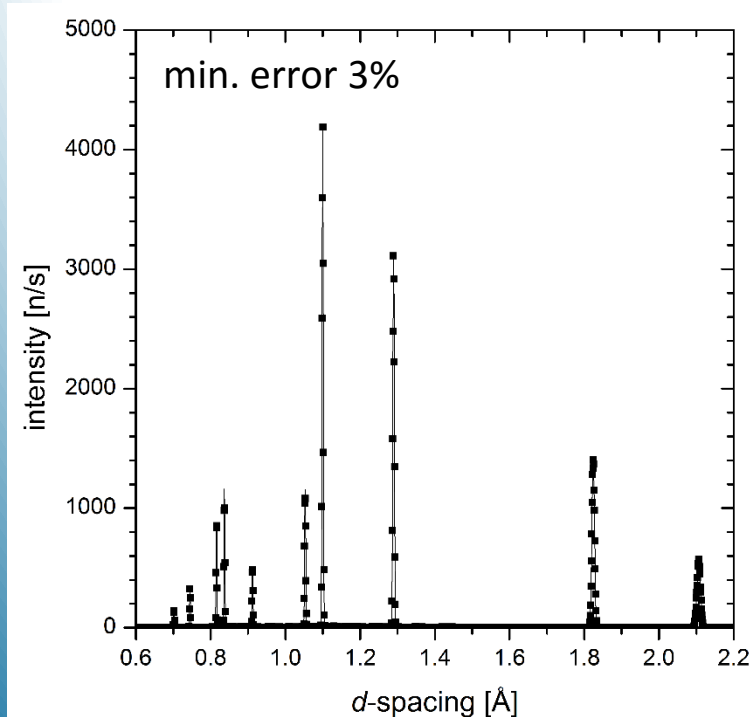
TRACE body is just an envelope which allows easy choice of tracing direction

Test with γ -Fe sample (Fe_Gamma.laz)

Conditions: *cylindrical sample:* 7 x 20 mm²
input slit: 5 x 10 mm², 50 mm before the sample
output radial collimator: 4 mm resolution (*fwhm*)
resolution mode: medium, $\Delta d/d = 0.3\%$
detector coverage: $2\theta = 75^\circ - 105^\circ$, $\phi = \pm 15^\circ$

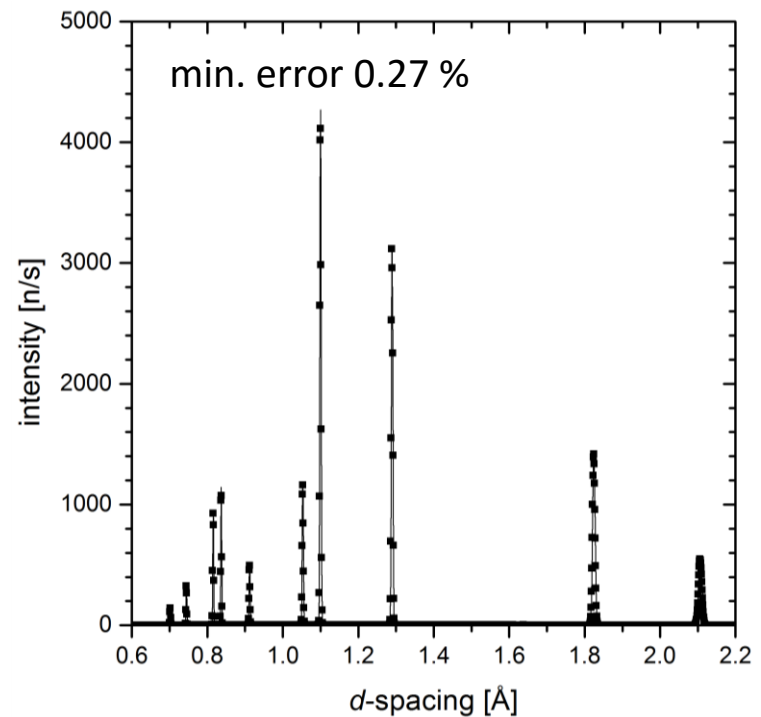
forward

trials: 5×10^9 , computing time: 12 h



reverse

trials: 5×10^8 , computing time: 4.2 h



Test with γ -Fe sample (Fe_Gamma.laz)

Simulation statistics (counts at the sample)

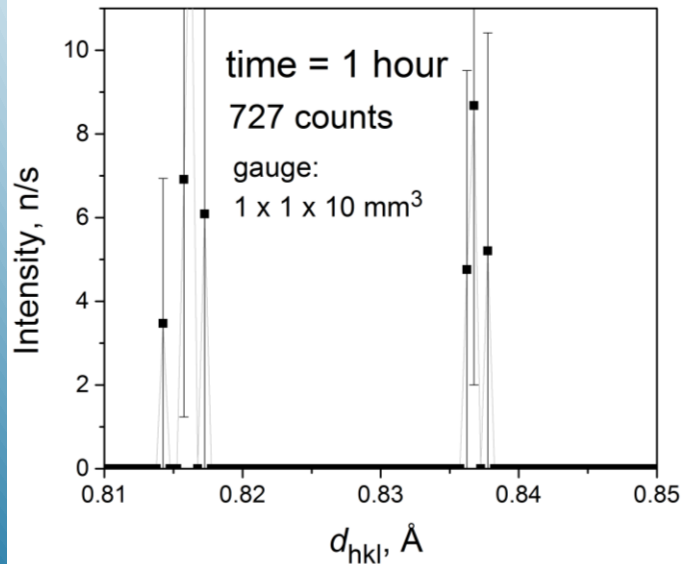
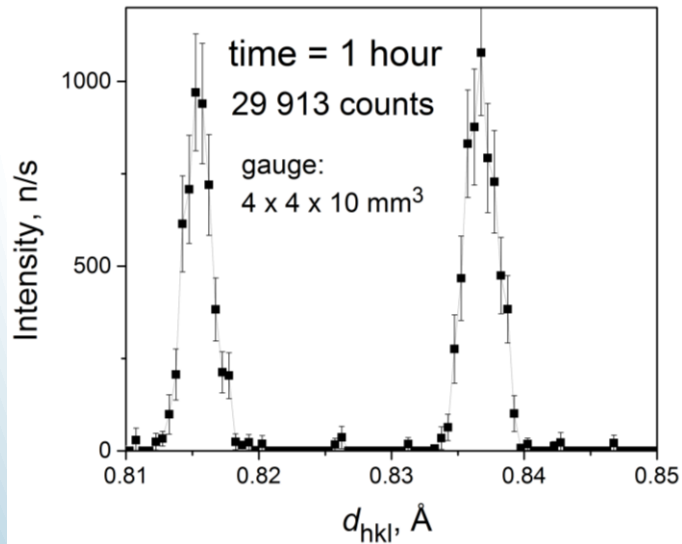
	forward	reverse	gain factor
Trials / 10^6	5000	500	
Counts / 10^6	0.18	24	
Efficiency [%]	0.0037	4.7	1300
Accuracy [%]	0.34	0.031	
Time [h]	11.95	4.15	
Time to 0.3 % accuracy [h] (*)	9.2	0.045	200

(*) corresponds to about 20 000 counts in the strongest peak, using SPLIT 20

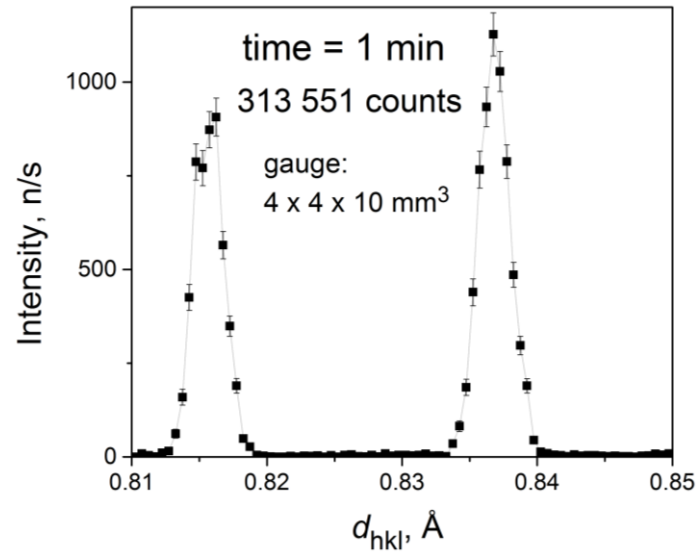
NOTE: The gain would be much higher for high resolution setup with small gauge volume of $\sim 10 \text{ mm}^3$
(typical for strain mapping experiments)

Test with γ -Fe sample (Fe_Gamma.laz)

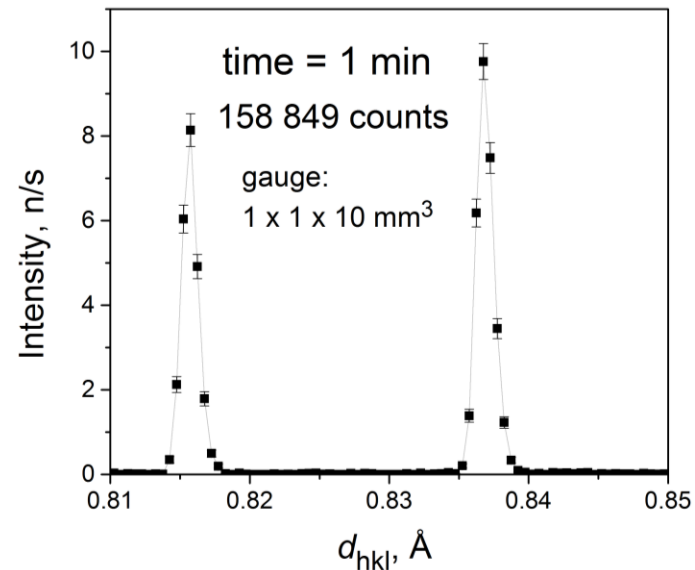
forward tracing



reverse tracing



medium
resolution



high
resolution

Drawbacks of the present implementation in McStas

- no “user friendly” solution
- requires construction of an inverted primary spectrometer
- all source components need to be modified (this is sometimes quite easy)
- monitors within the primary spec. do not show true flux
BUT: they could show “useful” neutrons = good for instrument optimization

Better solutions on the level of McStas compiler to be discussed ...

Advantages:

- ✓ gain about 2-3 orders of magnitude in CPU time
- ✓ speed independent of sample size !
- ✓ enables virtual experiments with small samples (e. g. strain scanning)
+ optimization of primary spec. based on scattering data

Thank you for your attention