SIMULATION OF INSTRUMENTS

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All you need is neutron seminar
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Outline

Why simulate neutron scattering instruments ?

How to simulate ?

Montecarlo method : Description

McStas and Monte Carlo

McStas in practice

Examples : IN8 and IN16b

Virtual experiment :

- Introduction and motivation
- Schematics and neutron-matter interaction
- Selected example

Why ?

I) Instrumentation :

Design

Upgrade

Assess improvement with a reference

→ Usual benchmark at sample : flux and divergence

→can place diagnostics anywhere and measure any quantity

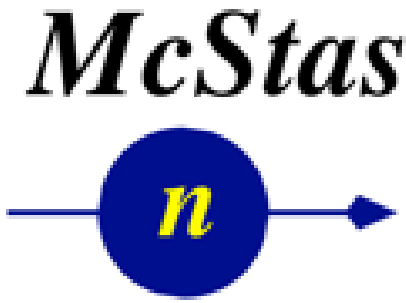
II) Physics : virtual experiment

Reproduce experimental data

Understand possible type of measurements

→ Usual benchmark at detector

Overview



A) Monte Carlo ray tracing simulations:

In particular McStas

Monte Carlo Simulation of neutron instruments

Originally made for TAS, triple axis spectrometry, but now includes all types of instruments and guides. About 90% of neutron scattering instrument went through a design process with Mcstas

B) Simulation of instrument resolution : Restrax, Phase space calculation

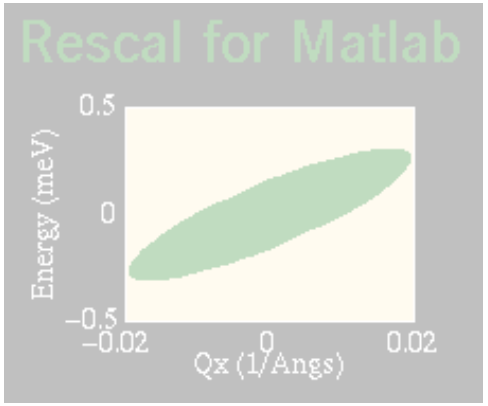
C) McNp : shielding, neutron filters,dosimetry

Simulation of instrument resolution

For three axis instruments and powder diffractometers :

Analytical approach :

individual neutron paths where resolution is represented by 4D ellipsoids → *Rescal*



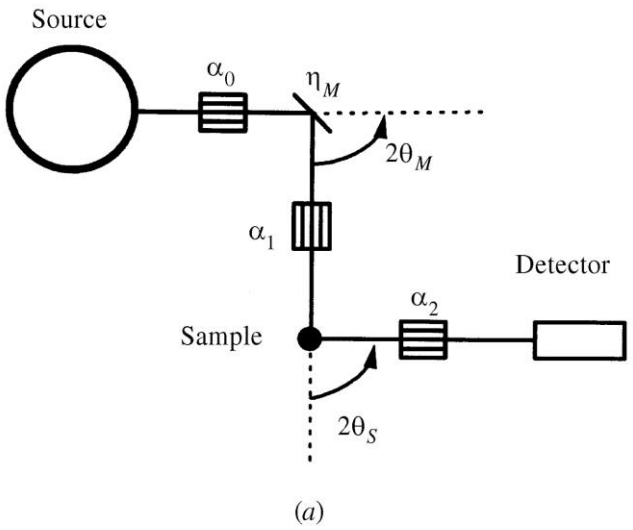
can also be combined with Montecarlo techniques → *Restrax*

RESTRAX

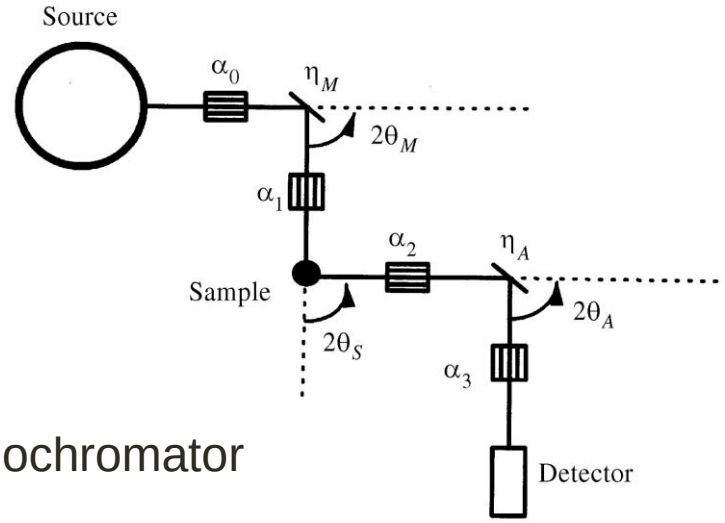
Phase space calculations

Phase space calculations

- *Goal* : obtain phase space diagrams of angular divergence and wavevector spread $\Delta\lambda$
- *Hypothesis* : rectangular elements
- *Application :* view the role of each beam element in the total instrument resolution -> better optimization of instrument and measurement



(a)



(b)

$\alpha_0, \alpha_1, \alpha_2, \alpha_3$ Half width at base of collimator

η_m Half width at base of monochromator

Phase space calculations

Neutron path with angle γ to mean direction : P is 1 if $|\gamma| < \alpha$, 0 otherwise

I) PSTR Primary spectrometer

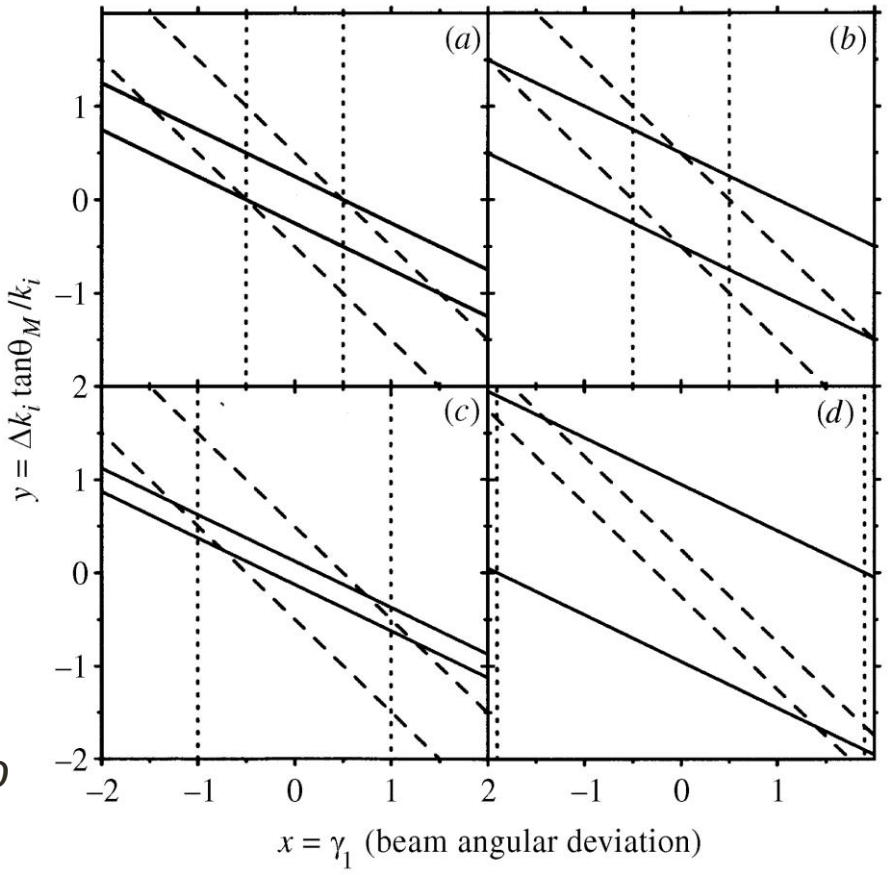
Neutron transmitted with angle γ_1 and wavector spread Δk_i with conditions :

$$\left| 2\frac{\Delta k_i}{k_i}\tan(\vartheta_m) + \gamma 1 \right| < \alpha_0$$

$$\left| \frac{\Delta k_i}{k_i}\tan(\vartheta_m) + \gamma_1 \right| < \eta_m$$

$$|\gamma_1| < \alpha_1$$

Intensity of the beam is proportional to the area of the Phase Space Transmission Region



Phase space calculations

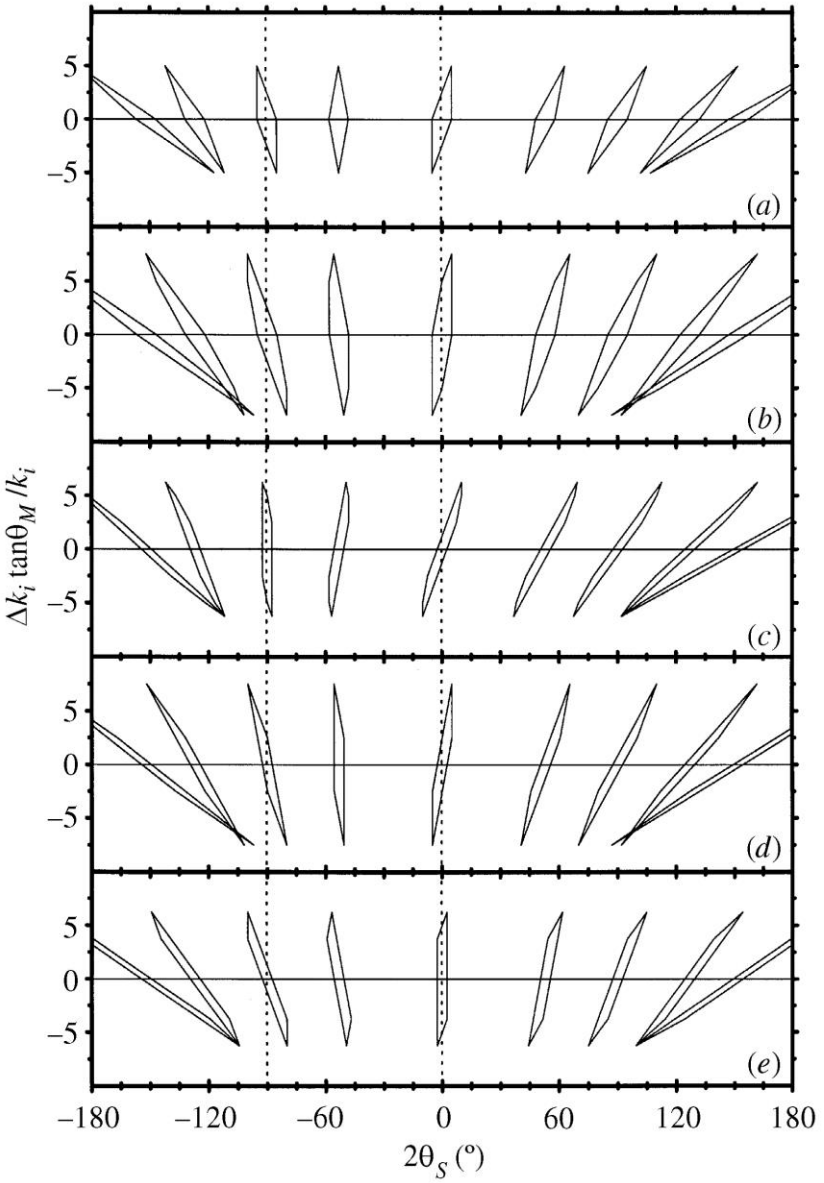
II) PSTR after the sample

Powder sample scatters elastically with Bragg peaks at angles $2\theta_s$:

Each phase space point :

$$(\gamma_1, \Delta k_i) -> (\gamma_2, \Delta k_f)$$

Scattering by powder sample :
- displaces PSTR along x axis and
- shears it parralell to x axis



Phase space calculations

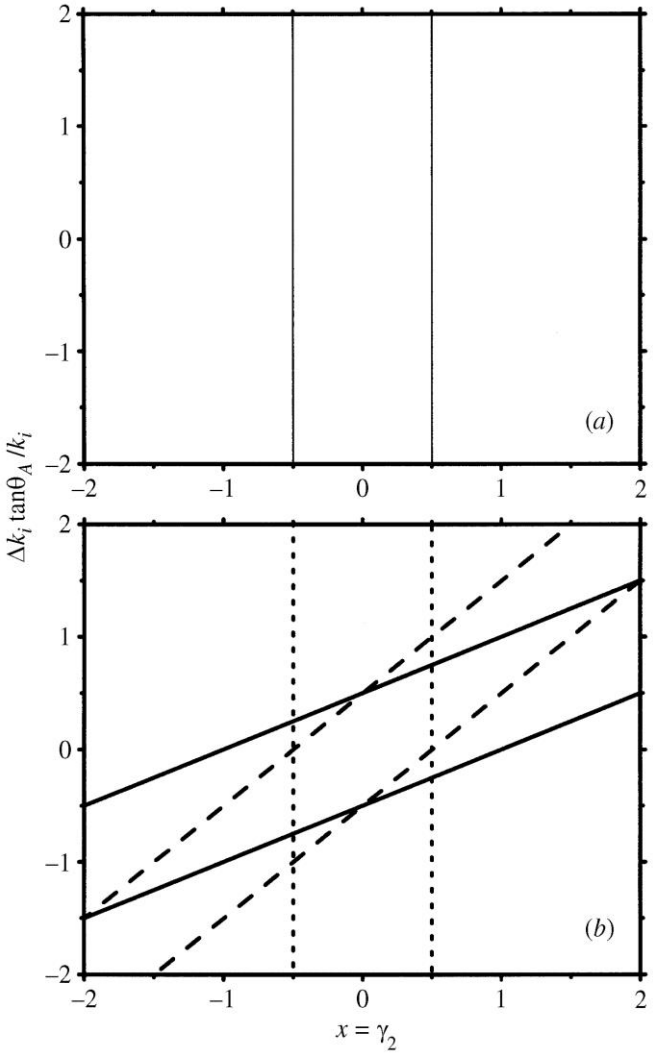
III) PSTR Secondary spectrometer and final PSTR

Powder diffractometer :
Collimator α_2 and detector
-> PSTR is 2 vertical lines

PSTR of a combination of elements = superposition of the PSTR of each element

- Maximum intensity is limited by the smallest PSTR
- PSTR of each element should match in shape and size

On powder diffractometer : optimize by reducing the shearing, for example with a large monochromator take off angle



Monte Carlo Simulation

Deterministic method

solve the integral transport equation for the average particle behavior

Monte Carlo method

simulates random individual particles and record some aspects of their average behavior.

Average behavior of the particles in the physical system is then inferred from the individual behavior.

-> MC well suited for complicated 3D and time-dependent problems

Random numbers, expectation and variance

A **random variable** :
- can take more than one value
- whose value cannot be predicted

But we can know the **distribution** of the variable.
For a continuous variable :

$$g(u)du = P[u < u' < u + du]$$

with $g(u)$ the **probability density function**

$G(u)$ the **integrated** distribution function has values from 0 to 1 and is given by :

$$G(u) = \int_{-\infty}^{u} g(x)dx$$

Expectation of a function $f(u')$: $E(f) = \int f(u)\, g(u)\, du$
if u' is **uniformly distributed** between a and b :

$$\boldsymbol{E(f) = \frac{1}{b-a}\int_{a}^{b} f(u)du}$$

Variance of a function : average squared deviation from the expectation

$$V(f) = E[f - E(f)]^{2.}$$

Law of large numbers

We choose n random numbers u_i with a uniform distribution from a to b. For each u_i, we evaluate $f(u_i)$.

Then :

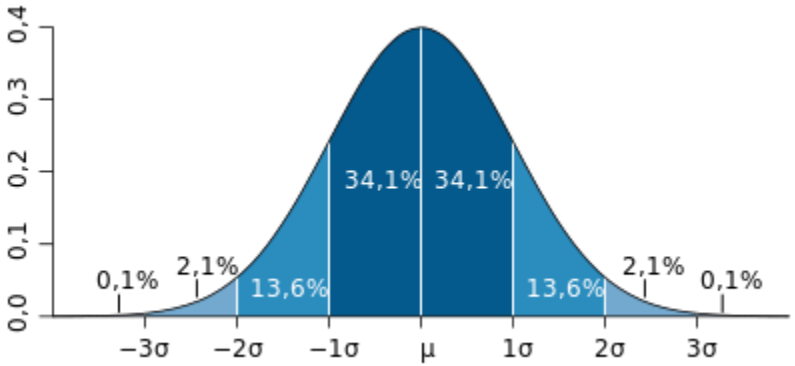
$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} f(u_i) = \frac{1}{b-a} \int_a^b f(u)\,du$$

Central limit theorem

The sum of a large number of independant random variable with finite expectation and variance is normally distributed, ie, a gaussian distribution

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-a)^2}{2\sigma^2}}$$

With a the expectation and σ^2 the variance



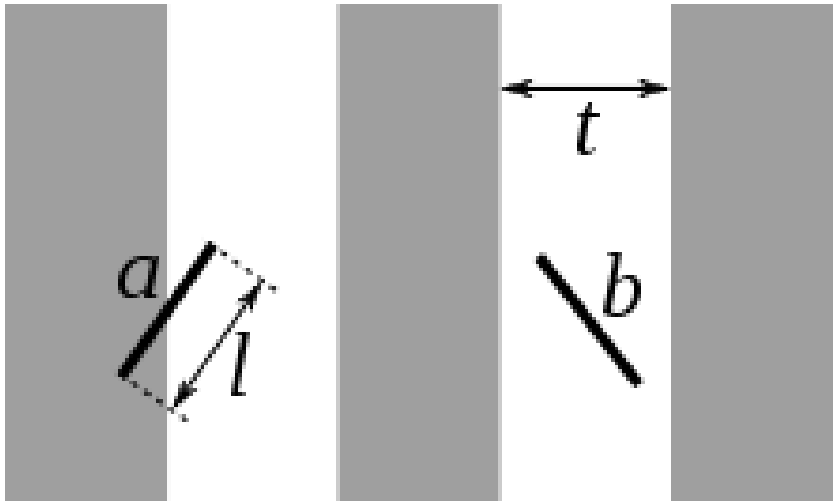
Let n independant x_i with expectation e_i and variance σ_i^2.
Then $S = \sum x_i$ with $E(S) = \sum e_i$ and variance $\sum \sigma_i^2$.
-> distribution is asymptotically gaussian

Useful for finite (but large n) to know how the MC estimate is distributed
-> asymptotically normally distributed

Hit or miss Monte Carlo: Buffon's needle to calculate π

Method :

- Pattern of parallel lines with distance t
- Throw randomly n needles of length l ($l \leq t$)
- Case a -> a hit
- Case b -> a miss



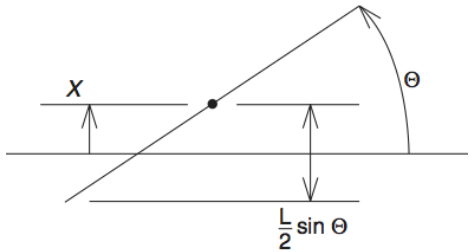
If n large, $\pi = \frac{l}{t} \frac{2\,n}{nb\ of\ hits}$

Probability of a hit :

Let x the distance from the center of the needle to closest line.

hit when $x \leq \frac{l}{2} \sin(\theta)$

We have $0 \leq \theta \leq \frac{\pi}{2}$ and $0 \leq x \leq \frac{t}{2}$



$$P\ (hit) = \frac{Area\ of\ a\ hit}{Total\ area} = \frac{\int_0^{\frac{\pi}{2}} \frac{l}{2} \sin\theta\ d\theta}{\frac{t\pi}{22}} = \frac{2\,l}{\pi t}$$

Variance reducing techniques

Incertainty on an MC integral : $\sigma = \sqrt{\frac{V(f)}{n}}$

I) Stratified sampling

Properties of Riemman integral : $\int_0^1 f(u)du = \int_0^a f(u)du + \int_a^1 f(u)du \, , 0<a<1$

1 : divide full integration interval in sub spaces
2 : in j^{th} subspace of length {j} : choose n_j points
3 : do partial sum in each sub space
4 : add partial sums weighted by $\{j\}/n_j$

To reduce the variance -> equal length and equal number of points

Difference in variance for 2 regions is then :

$$D(s^2) = \frac{1}{n}\left|\int_{(1)} f(x)dx - \int_{(2)} f(x)dx\right|^2$$

Variance reducing techniques

II) Importance sampling

Large variation in values of f -> large uncertainty in MC estimate

Idea : choose large number of points in sampling space where f is large and compensate by reducing the function value in that region

Mathematically :

$f(x)dx -> f(x)\, dG(x)/g(x)$ and so the variance $V(f) -> V\left(\frac{f}{g}\right)$

We choose points according to $G(x)$ the integrated distribution function and then weight $f(x)$ by $\frac{1}{g(x)}$

$g(x) = dG(x)/dx$, the probability density function

Extension : adaptive importance sampling

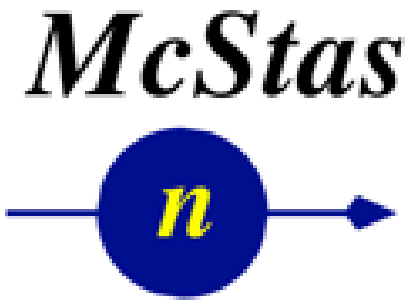
Montecarlo technique and simulation strategy

Behavior of a neutron scattering instrument :

a complicated integral over all the relevant parameters, not solvable analytically

Let's see how Monte Carlo is applied for intrument simulation in McStas :

- Trick 1: Ray tracing simulation and neutron weight
- Trick 2 : adaptive importance sampling
- Trick 3 : stratified sampling



Ray tracing simulation and neutron weight factor

- Simulation neutron by neutron : only a very small fraction will ever be detected

→ neutron weight factor for each simulated neutron ray and do weight adjustement according to the path.

The final weight p after n elements is :

$$p = p_0 \prod_{j=1}^{n} \pi_j$$

Simple Example : simulate an optical component with 10% reflectivity :
-> All rays are allowed through but each weight p is multiplied by 0.1

Neutron ray/package in McStas:

Weight (p):
Coordinates (x,y,z)
Velocity (v_x,v_y,v_z)
Spin (s_x,s_y,s_z)
Time (t)

Ray tracing simulation and neutron weight factor

- Monte Carlo simulation of an element :

When a MC choice is performed -> adjust the neutron weight so that probability of this choice matches the physical properties

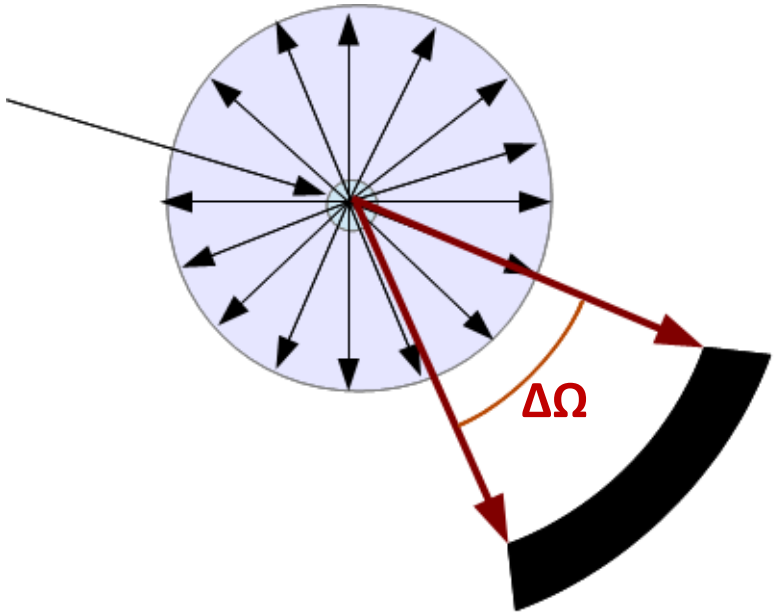
$$f_{MC}\,\pi_j = P$$

MC choice of transmitting the ray

Weight factor

Probability to transmit the real neutron

Adaptive Importance sampling



Importance sampling : Focus only on the interesting directions

Ex : sample scatters isotropically over 4π but interesting direction over solid angle ΔΩ :

$$f_{MC}(\Delta\Omega) = 1$$
$$P(\Delta\Omega) = \Delta\Omega / 4\pi$$

Adaptive importance sampling : interesting directions determined during the simulation, leading to a gradual change of the focusing

Stratified sampling

- Partitioning the event distribution into representative subspaces that are then sampled individually

→ Instead of N events : define D partition and shoot r=N/D events in each

Can be combined with adaptive sampling to represent interesting direction

Used in McStas for repeting events such as virtual sources

Note on accuracy of MC simulation

Accuracy of the estimates in function of the space dimension d and the number of events N.

exact expression depends on the random distribution, but for large n the estimate of the relative error is $\frac{1}{\sqrt{N}}$ (central limit theorem)

Mcstas has d=10 parameters

(weight,position, velocity,spin and time)

Records	Accurarcy
10^3	10 %
10^4	2.5 %
10^5	1 %
10^6	0.25 %
10^7	0.05 %

Simulation of instruments : Components

Add components that transform the neutron ray parameters (weight,…) to model instruments

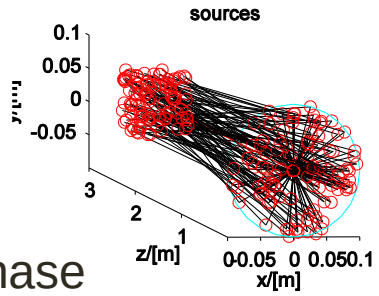
Sources (neutrons)
Continuous (reactor), Pulsed

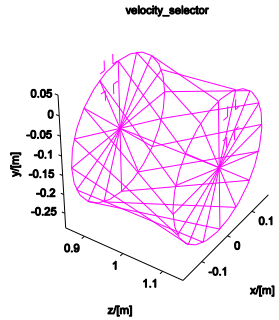
Moving optics
Choppers (disk and Fermi), velocity selectors, phase space transformers

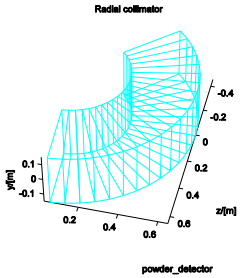
Static optics
Guides, mirrors, benders, lenses, collimators, slits, filters, monochromators

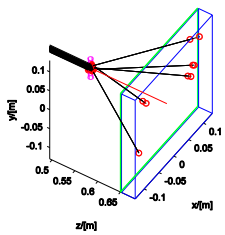
Samples/materials
Single crystals, liquids, gas, polymers, hard spheres

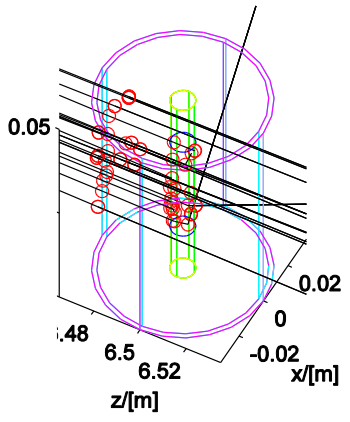
Detectors
Histogram and event monitors, gas detectors











McStas in practice

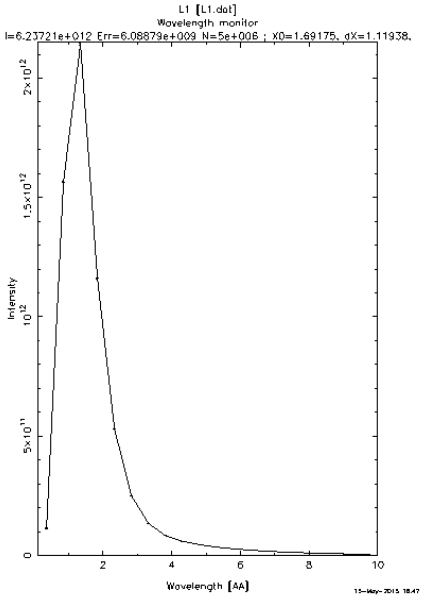
Instruments are defined from a text file. General syntax is based upon C.
Basic syntax:

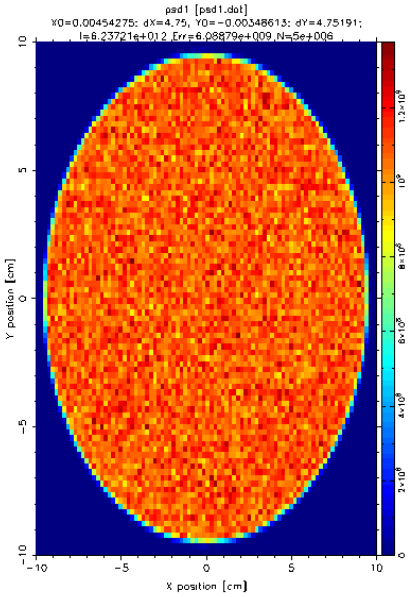
```
DEFINE INSTRUMENT name(parameter1=value1, …)

DECLARE %{ /* global variables */
%}

INITIALIZE %{ /* code executed when starting */
%}

TRACE    /* sequence executed for each neutron event */
COMPONENT InstanceName=component(parameters...)
AT (position) RELATIVE reference
ROTATED (orientation) RELATIVE reference
...
END
```

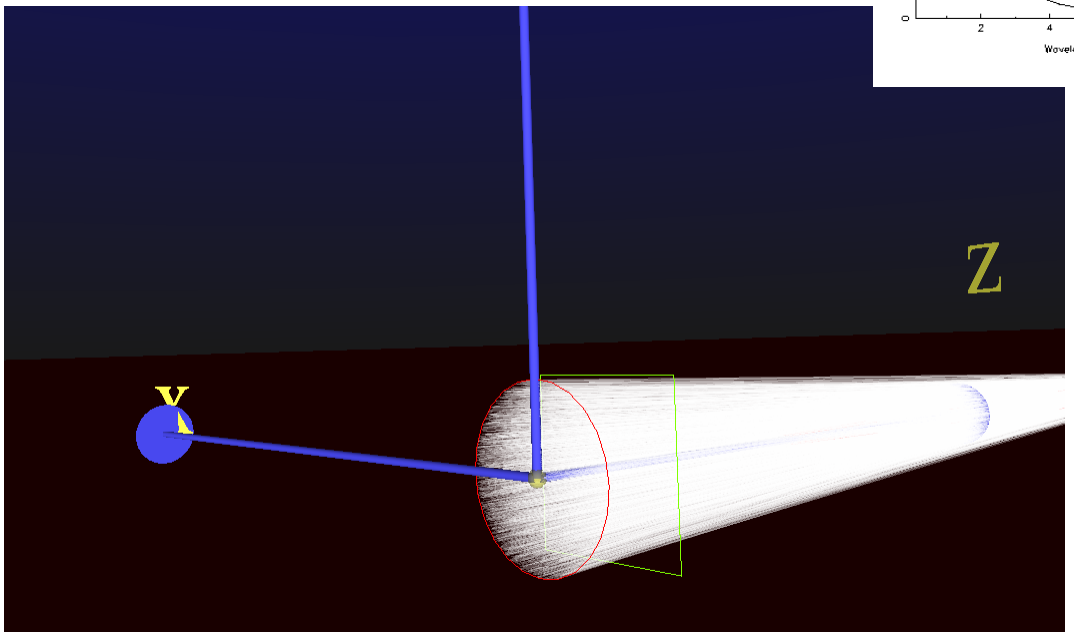
Let's first have some (thermal) neutrons

COMPONENT **Origin = Arm()**
AT (0,0,0) ABSOLUTE

COMPONENT source =
Source_gen(radius=0.1,Lmin=0.1,Lmax=10,T1=683.7,I1=0.5874e+13,T2=257.7,I2=2.5099e+13,T3=16.7,I3=1.0343e+12,focus_xw=0.05,focus_yh=0.05,dist=2)
AT (0,0,0) RELATIVE Origin







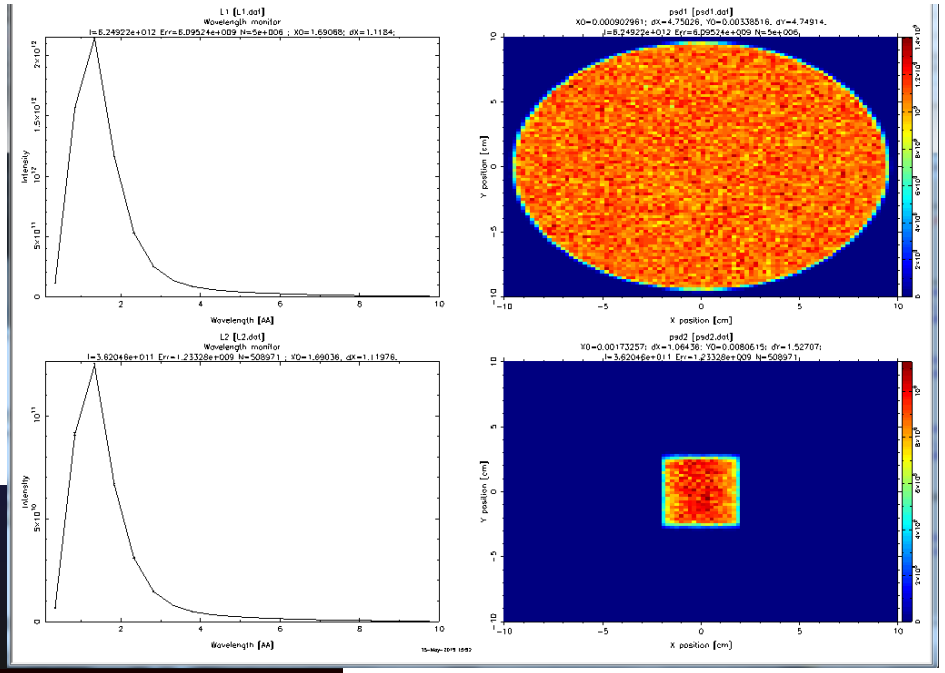
And monitors

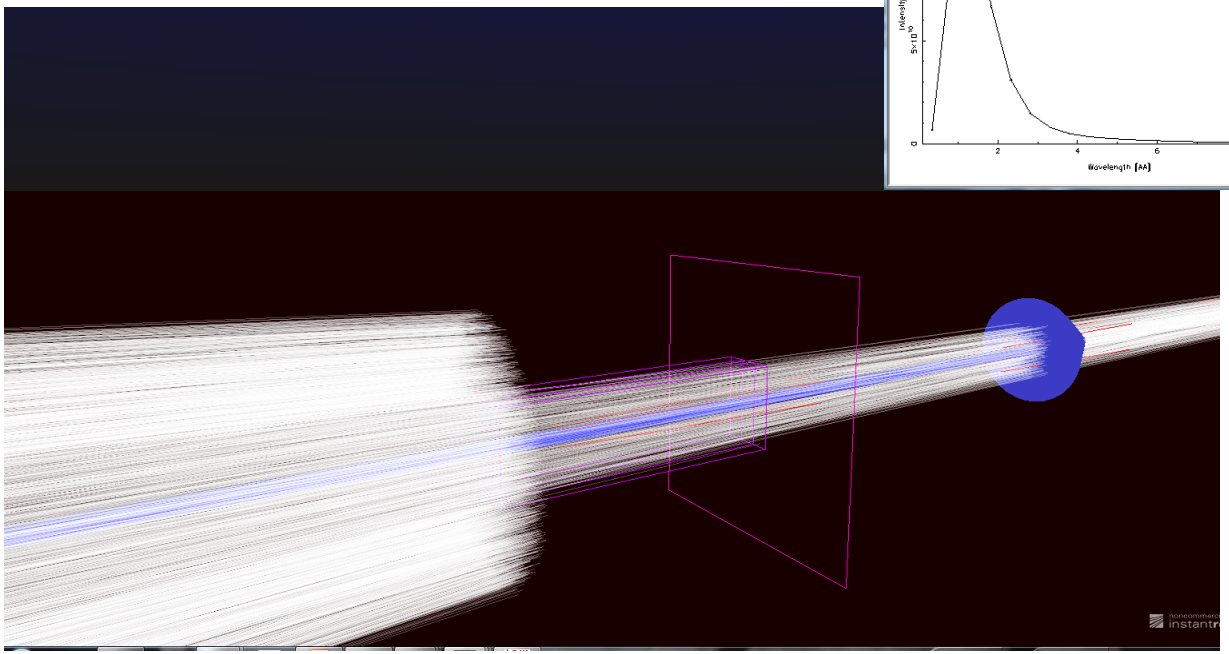
COMPONENT L1 = L_monitor(
filename = "L1.dat", xmin = -0.1, xmax = 0.1, ymin = -0.1,
ymax = 0.1, Lmin = 0.1, Lmax = 10,restore_neutron=0)
AT (0, 0, 0.1) RELATIVE Origin

COMPONENT psd1 = PSD_monitor(
filename = "psd1.dat", xmin = -0.1, xmax = 0.1, ymin = -0.1,
ymax = 0.1,restore_neutron=0)
AT (0, 0, 0.1) RELATIVE Origin

Let’s add collimation

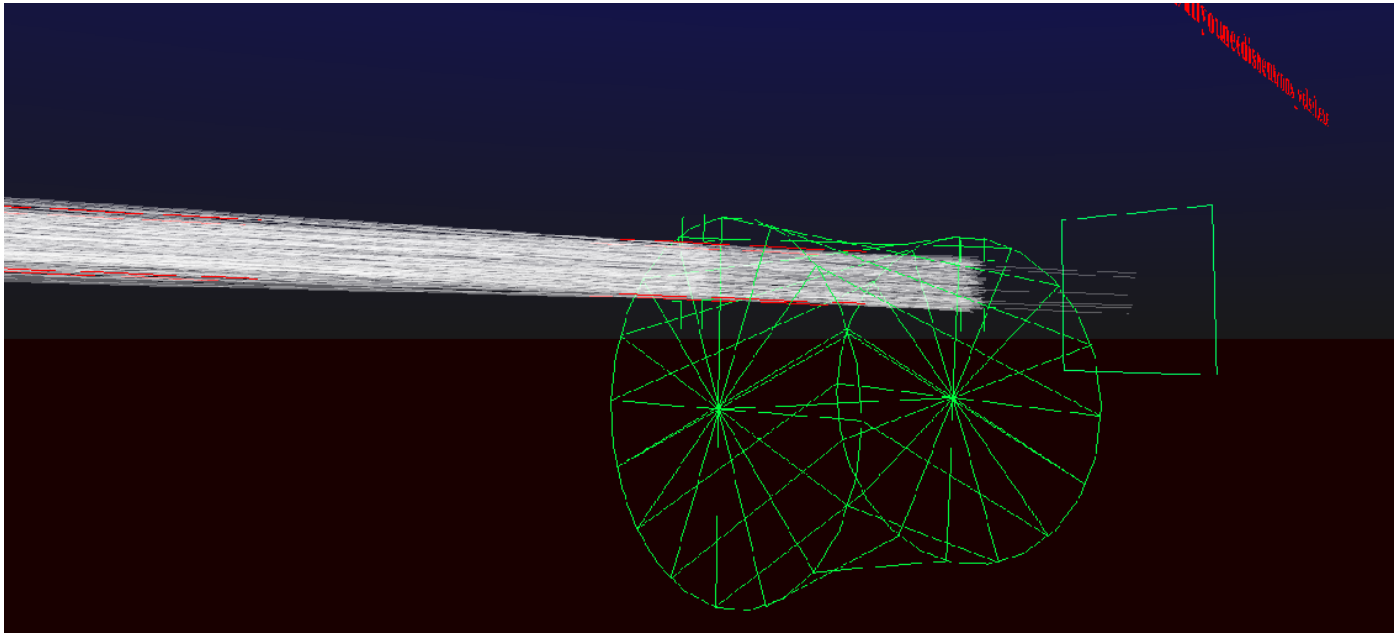
COMPONENT collimator = Collimator_linear
(length = 0.2, divergence = coll_div, xmin = -0.02, xmax = 0.02, ymin = -0.03, ymax = 0.03)
AT (0, 0, 0.4) RELATIVE Origin





Let's try a velocity selector

COMPONENT velocity=V_selector(xwidth=0.03, yheight=0.05, zdepth=0.30, radius=0.12, alpha=48.298, length=0.25, d=0.0004, nu=1500,nslit=72)
AT (0,0,2) RELATIVE Origin

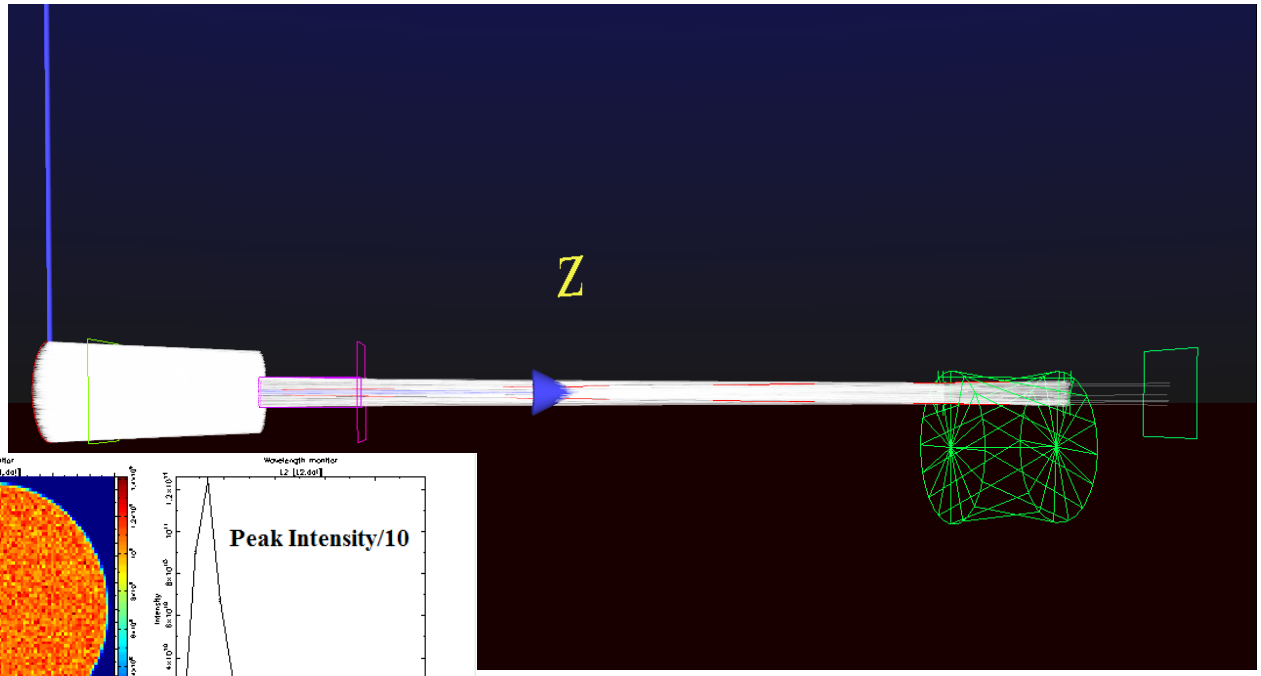


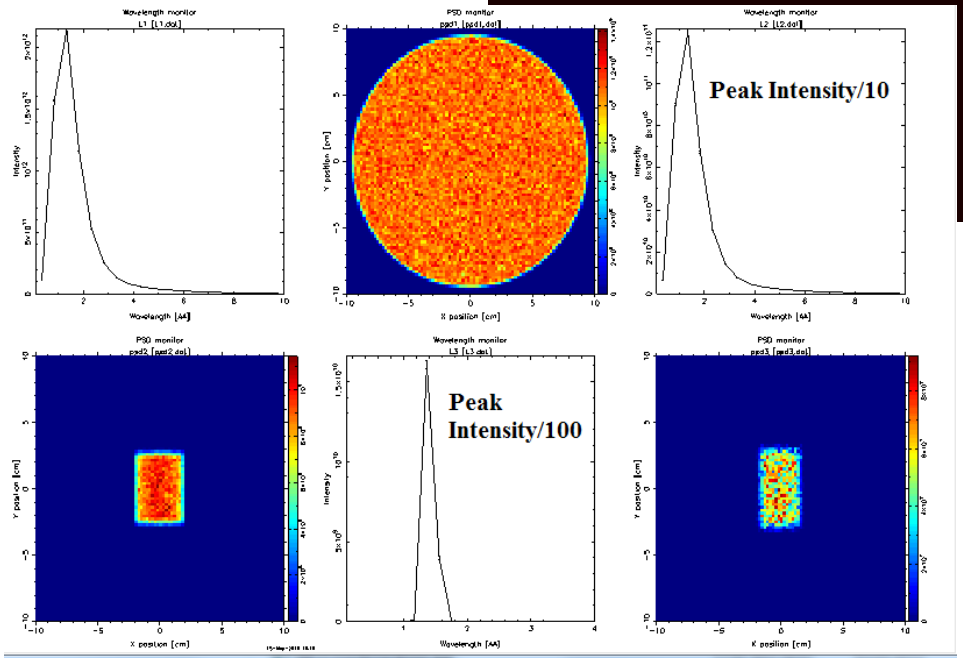
Note :

- The flight path of the neutron through the curved slits is not simulated
- Allow transmittance of neutron ray with velocity $v = \frac{wL}{\alpha}$ with w the rotation speed (in rpm), L the length and α the twist angle

Finally, add a detector

Note :
Detectors are equivalent to monitors in Mcstas



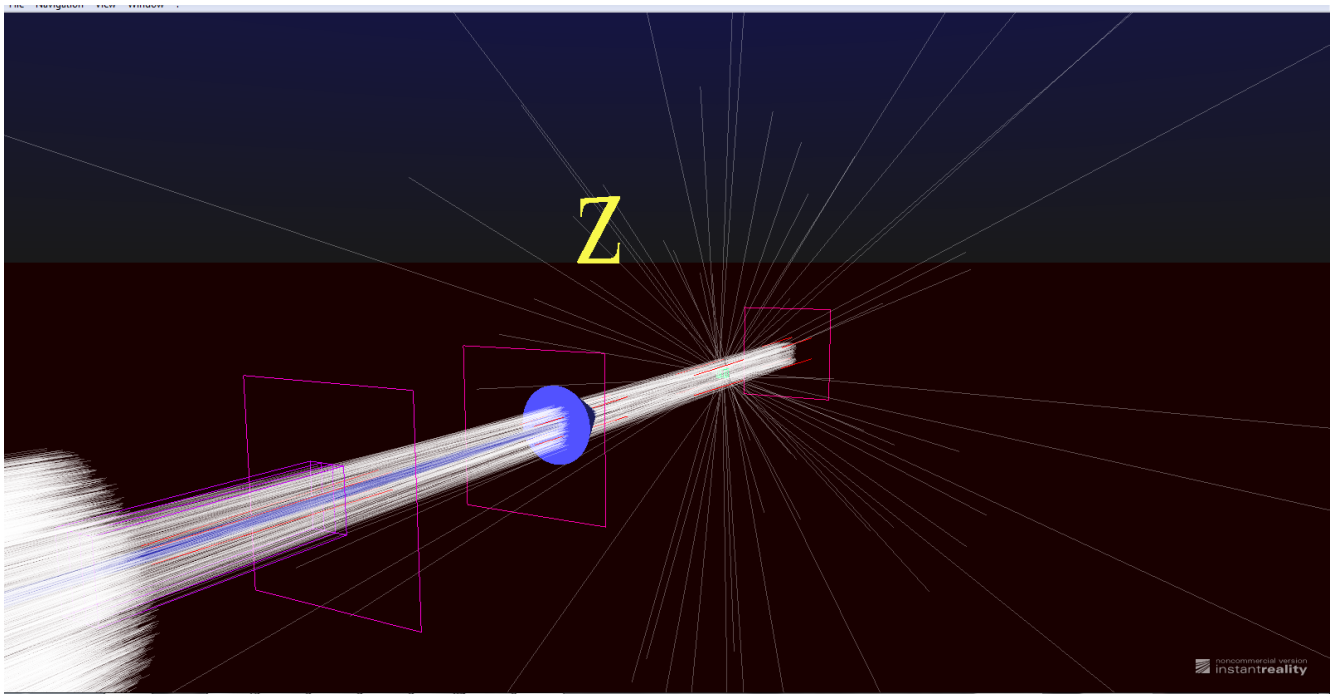


Choice of $nu = 1500\ Hz$:
We obtain $\lambda = 1.44$ Å

Now let's go back and try a sample

The velocity selector is removed and an anular vanadium sample is added

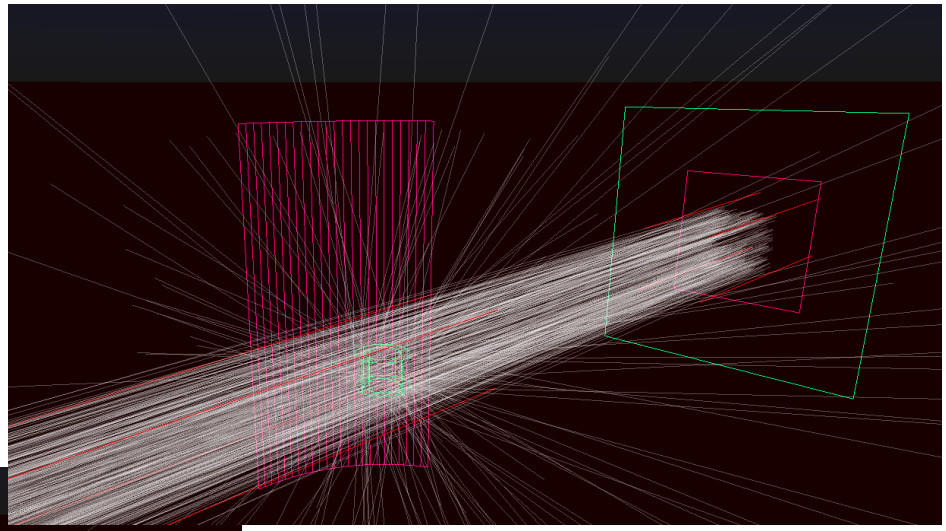
COMPONENT vana =
Incoherent(sigma_abs=5.08,sigma_inc=5.08,Vc=13.827
radius = 0.012, thickness = 0.004,yheight=0.015)
AT (0,0,1.5) RELATIVE Origin

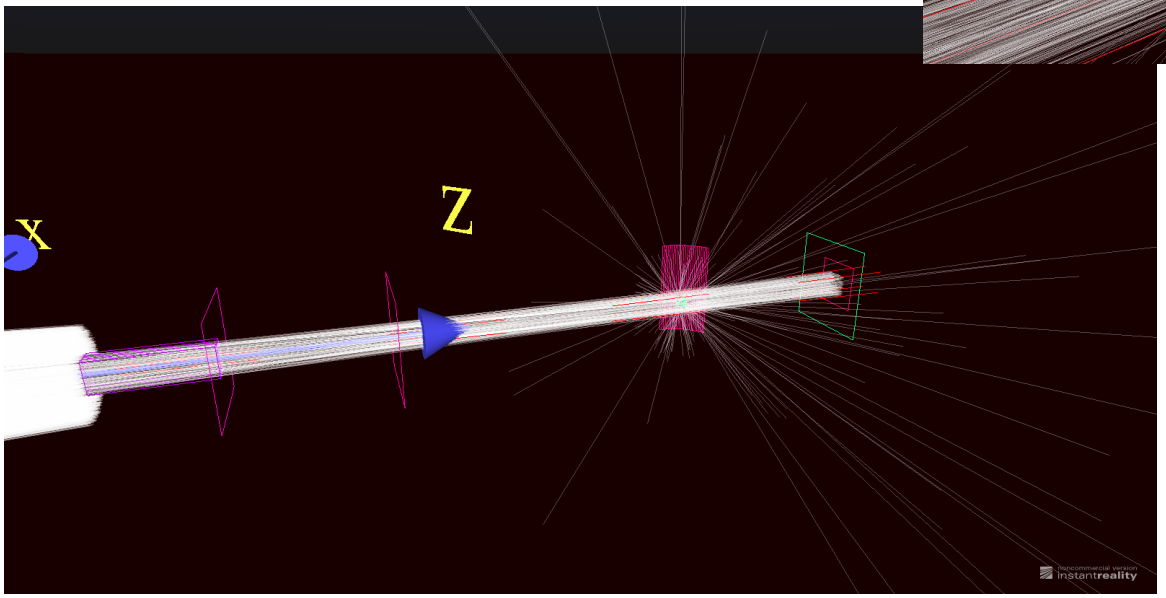


Finally, a banana detector and a beam stop

COMPONENT mydetector=Monitor_nD(xwidth = 0.2, yheight = 0.2, zdepth = 0, options = "banana, theta limits=[30,90], bins=120, y")

AT (0, 0, 0) RELATIVE vana

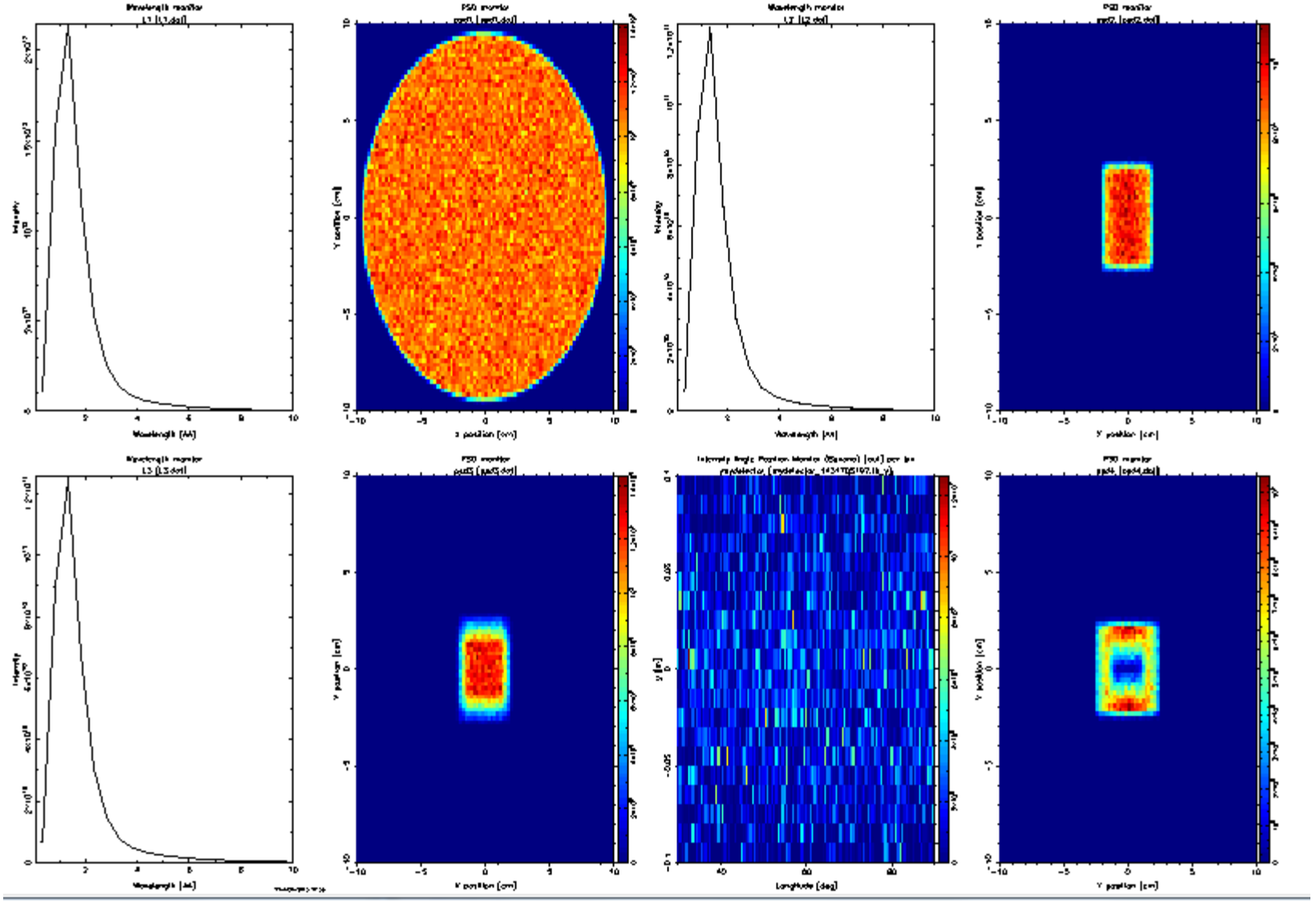




COMPONENT stop = Beamstop (xmin = -0.05, xmax = 0.05, ymin = -0.05, ymax = 0.05)

AT (0, 0, 0.4) RELATIVE vana

Results on monitors



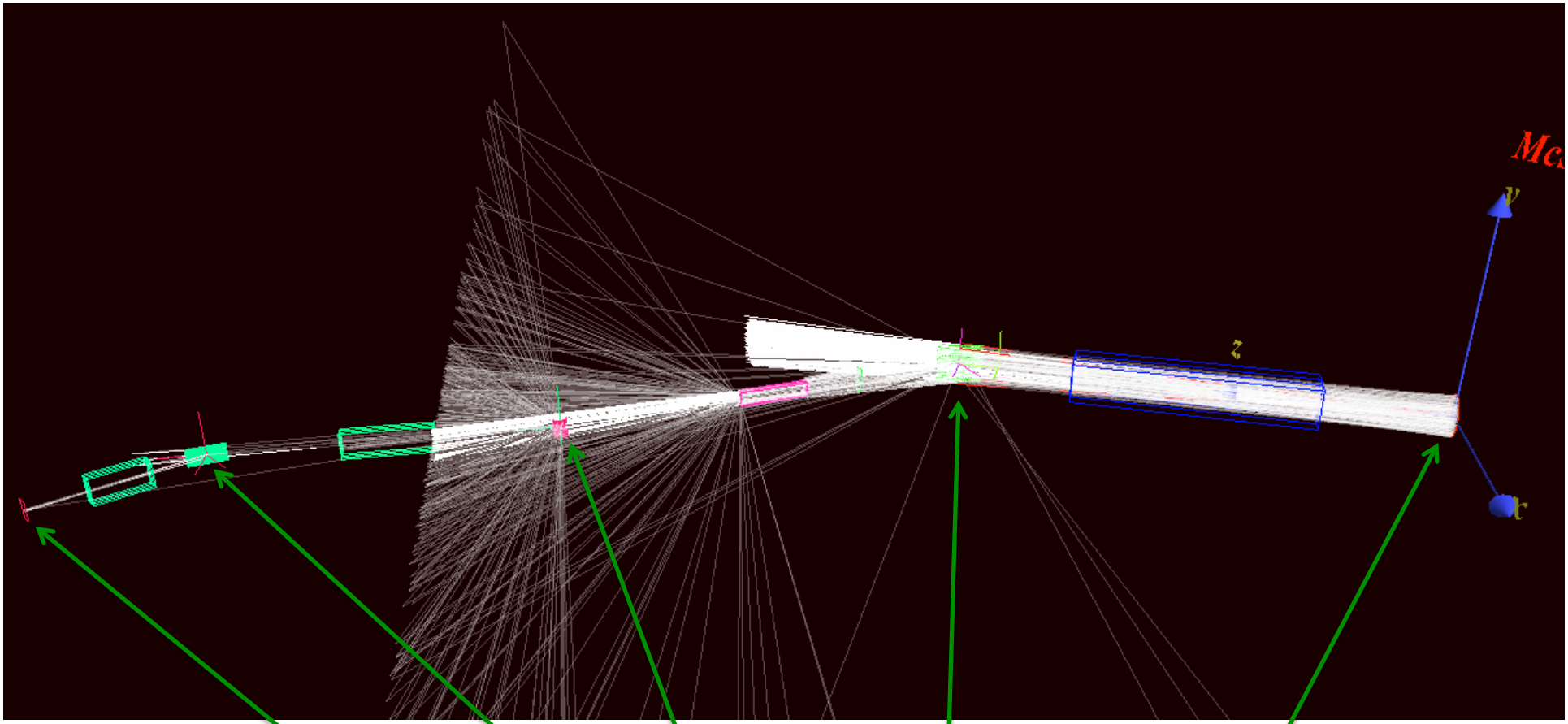
Next : Some examples of simulation of ILL instruments and discussion of virtual experiments

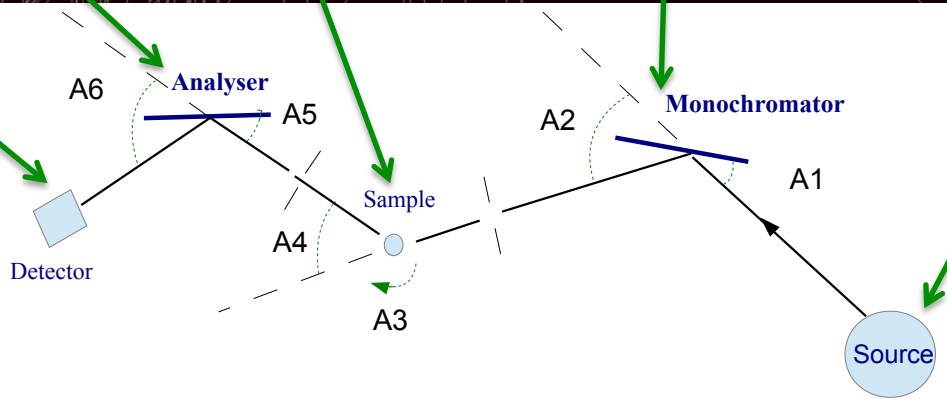
Two examples of simulated instruments

- All you need is neutrons -

Marco Grimaldo, Diane Lançon

IN8


z
y
x


A6
Analyser
A5
A2
Monochromator
A1
Sample
A4
Detector
A3
Source

IN8

Definition file of IN8

Edit: ILL_H10_IN8.instr

File Edit Search View Insert

```
*******************************************************************************/

DEFINE INSTRUMENT ILL_H10_IN8(
  KF=5, KI=0, QM=0.5, EN=0, verbose=1,
  WM=0.233, HM=0.197, RMH=-1, RMV=-1, DM=1.807, NHM=15, NVM=15,
  WA=0.16, HA=0.08, RAH=-1,   RAV=-1, DA=2.087, NHA=15, NVA=15,
  L1=2.3,
  ALF1=60, ALF2=60, ALF3=60, ALF4=60,
  BET1=120, BET2=120, BET3=120, BET4=120
)

TRACE

REMOVABLE COMPONENT Origin=Progress_bar()
AT (0,0,0) ABSOLUTE

/* a flat constant source: tube H10 is twice as brilliant as H12 */
REMOVABLE COMPONENT Source = Source_gen(
  radius  = 0.10,
  dist = machine_hkl.l1,
  focus_xw = fabs(WM*sin(machine_real.a1*DEG2RAD)), focus_yh = HM,
  T1=683.7,I1=0.5874e+13,T2=257.7,I2=2.5099e+13,T3=16.7 ,I3=1.0343e+12,
  E0 = machine_hkl.ei,
  dE = machine_hkl.ei*0.03)
AT (0,0,0) ABSOLUTE

REMOVABLE COMPONENT SC1 = Collimator_linear(
  xmin =-WM/2, ymin =-HM/2,
  xmax = WM/2, ymax = HM/2,
  length = machine_hkl.l1/2,
  divergence=ALF1,
  divergenceV=BET1)
WHEN (ALF1 && BET1)
AT (0, 0, machine_hkl.l1/4) ABSOLUTE

REMOVABLE COMPONENT Guide_out=Arm()
AT (0, 0, machine_hkl.l1-0.2) ABSOLUTE

%include "templateTAS.instr"

END
```

Line: 1 of 166 total, Column: 0

Generic TAS

Put source at (0,0,0)

```
TRACE
/* Source description */

REMOVABLE COMPONENT Origin=Progress_bar()
AT (0,0,0) ABSOLUTE

/* a flat constant source */
REMOVABLE COMPONENT Source = Source_gen(
  radius  = 0.10,
  dist = machine_hkl.l1,
  focus_xw = fabs(WM*sin(machine_real.a1*DEG2RAD)), focus_yh = HM,
  T1 = 683.7, I1 = 0.5874e13, T2 = 257.7, I2 = 2.5094e13, T3 =  16.7, I3 = 0.10343e13,
  E0 = machine_hkl.ei,
  dE = machine_hkl.ei*0.03)
AT (0,0,0) ABSOLUTE
```

IN8

Generic TAS

Define an “arm”
starting from the origin

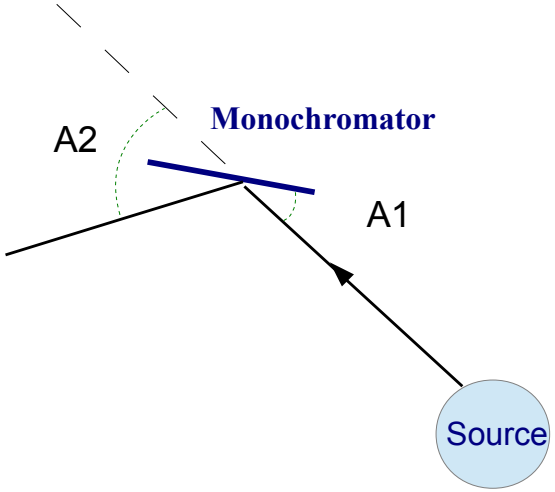
```
REMOVABLE COMPONENT Guide_out=Arm()
AT (0, 0, machine_hkl.l1-0.2) ABSOLUTE

COMPONENT Mono_Cradle = Arm()
  AT (0, 0, 0.2) RELATIVE PREVIOUS
```

Put monochromator along the arm
using RELATIVE coordinates

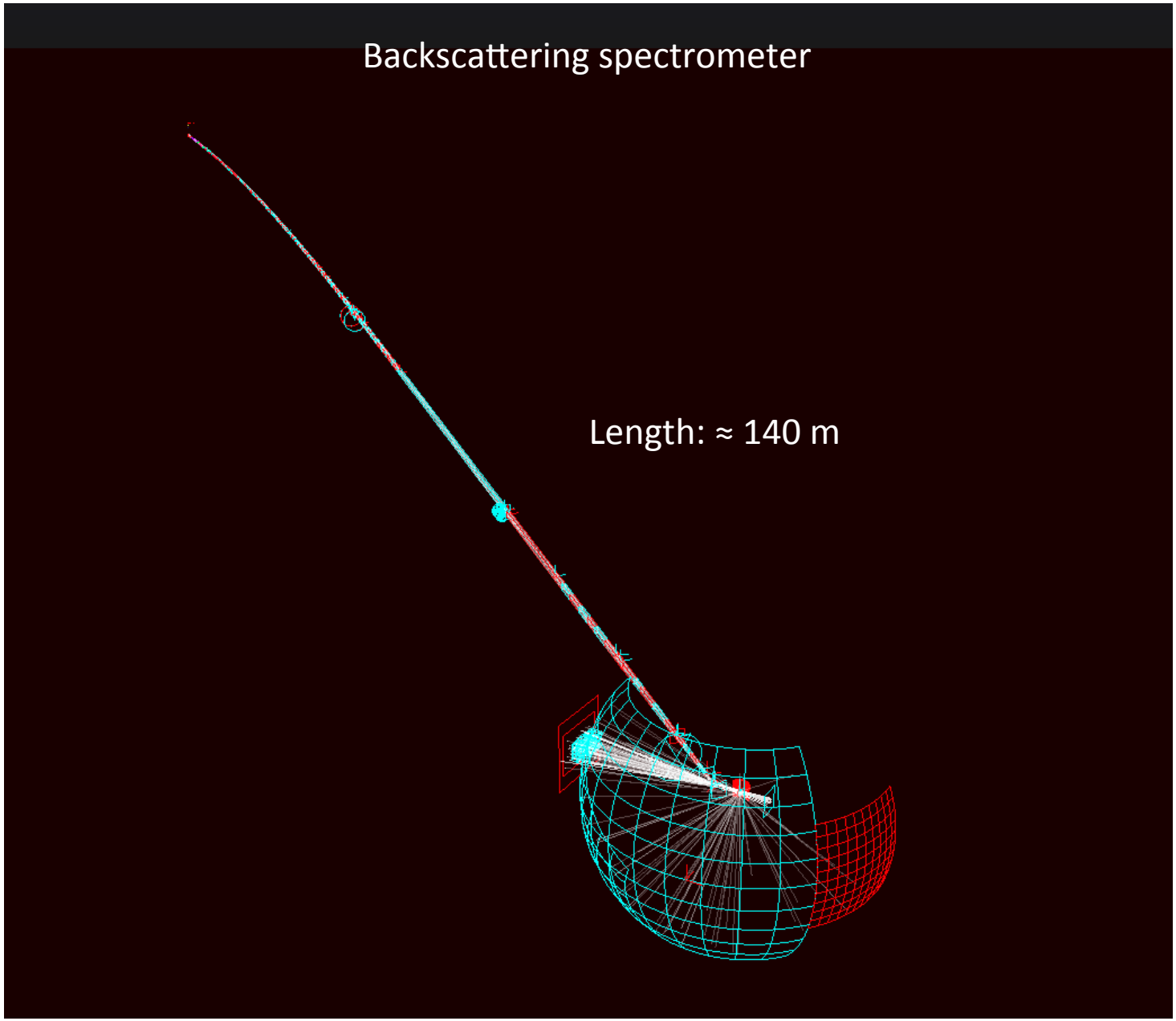
```
SPLIT COMPONENT PG1Xtal = Monochromator_curved(
  width  = WM,
  height = HM,
  NH=NHM, NV=NVM,
  RV=machine_real.rmv, RH=machine_real.rmh,
  DM=machine_hkl.dm, mosaich = machine_hkl.etam, mosaicv = machine_hkl.etam,
  r0 = (fabs(machine_hkl.dm-3.355) < 0.2 ? 1: 0.7),
  reflect=(fabs(machine_hkl.dm-3.355) < 0.2 ? "HOPG.rfl" : ""))
AT (0, 0, 0) RELATIVE Mono_Cradle
ROTATED (0, machine_real.a1, 0) RELATIVE Mono_Cradle
```

Define another “arm”
RELATIVE to the monocrhomator
ROTATED by the angle A2

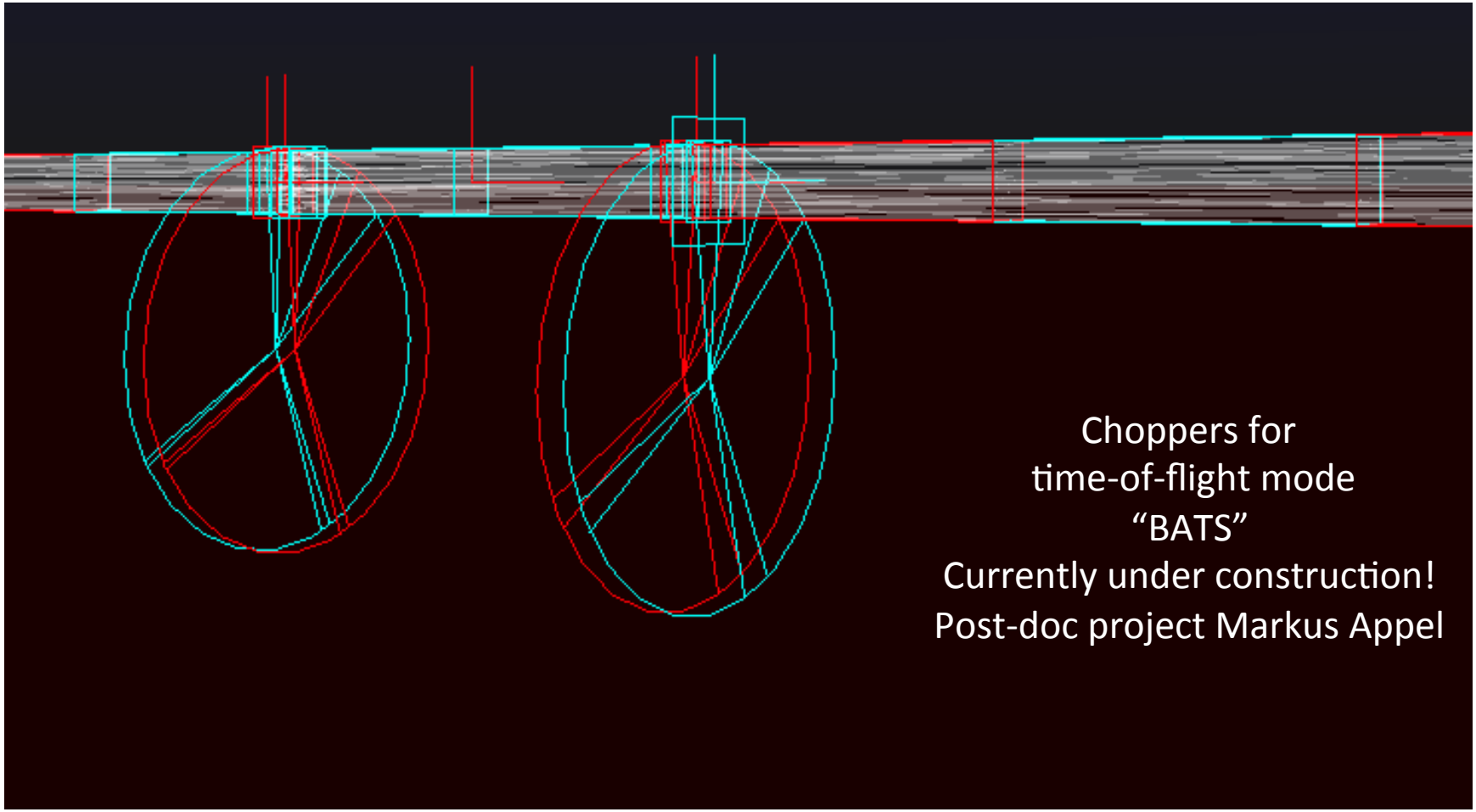
```
/*                          on mono, pointing towards sample */
COMPONENT Mono_Out = Arm()
  AT (0,0,0) RELATIVE Mono_Cradle
  ROTATED (0, machine_real.a2, 0) RELATIVE Mono_Cradle
```



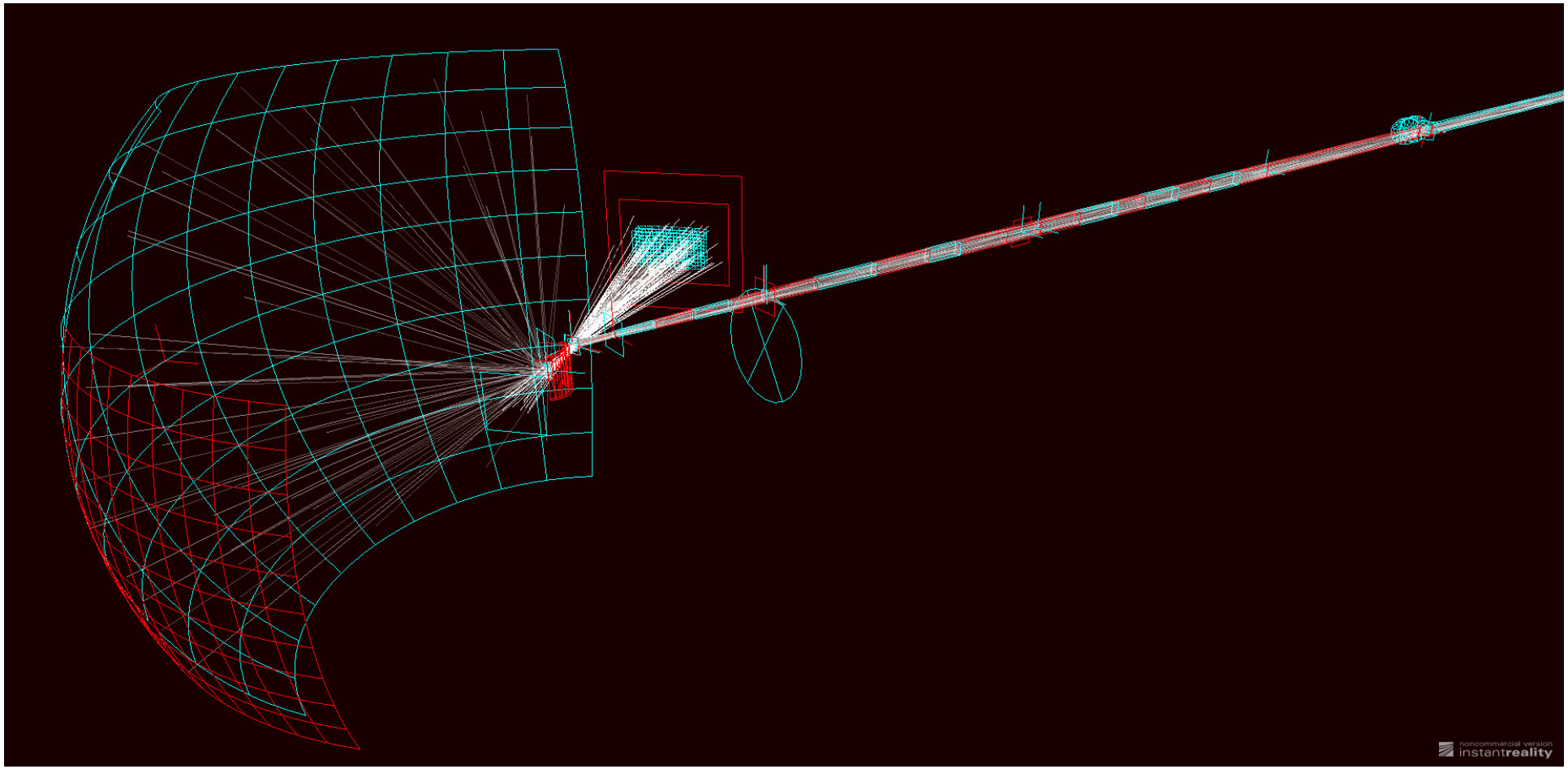
IN16B – Full view



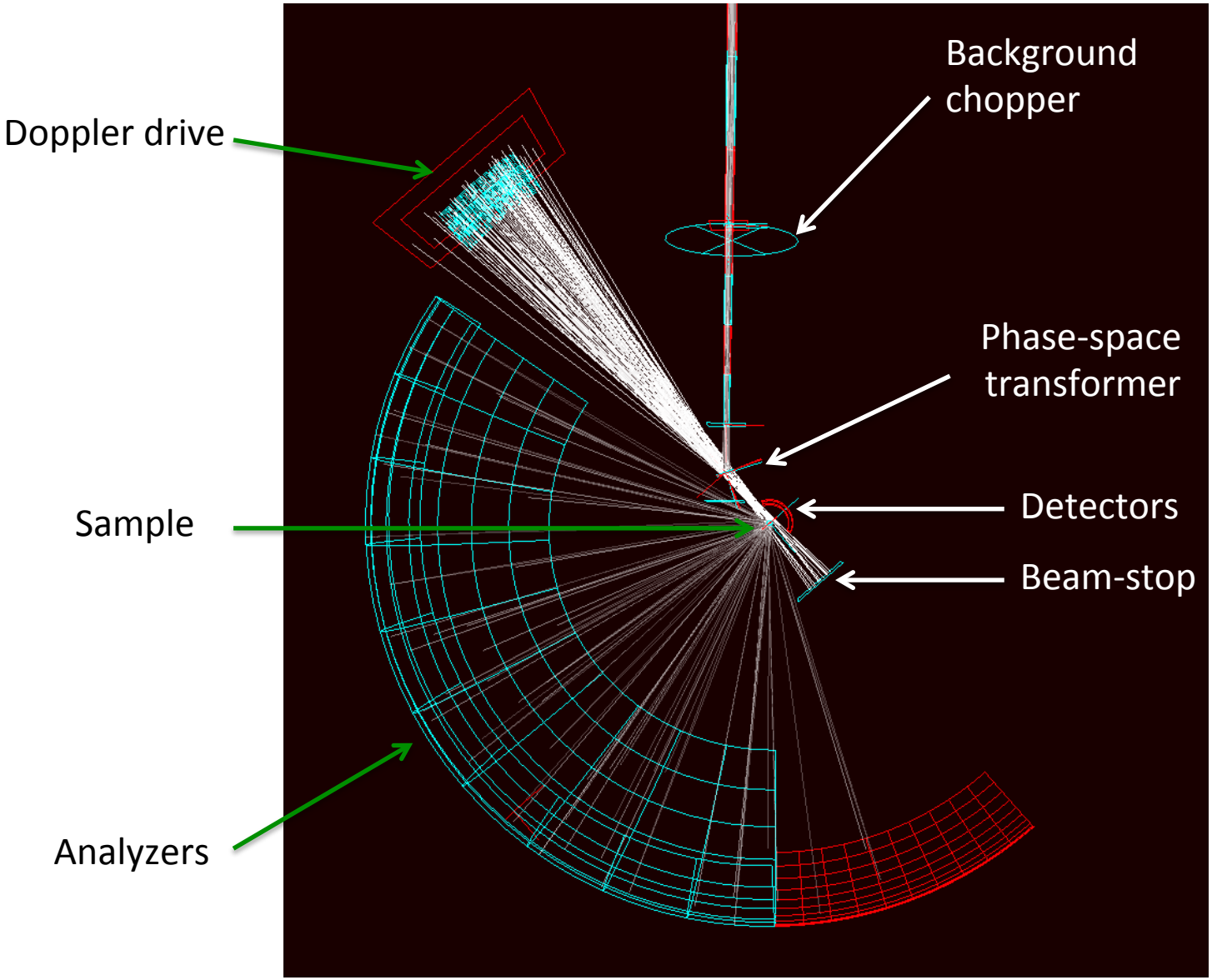
IN16B – BATS choppers



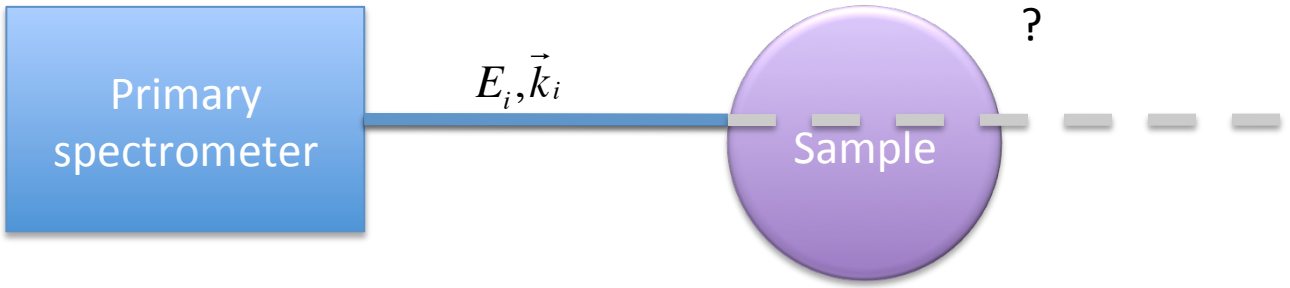
IN16B – side view



IN16B – top view



Virtual experiments with McStas



- All you need is neutrons -

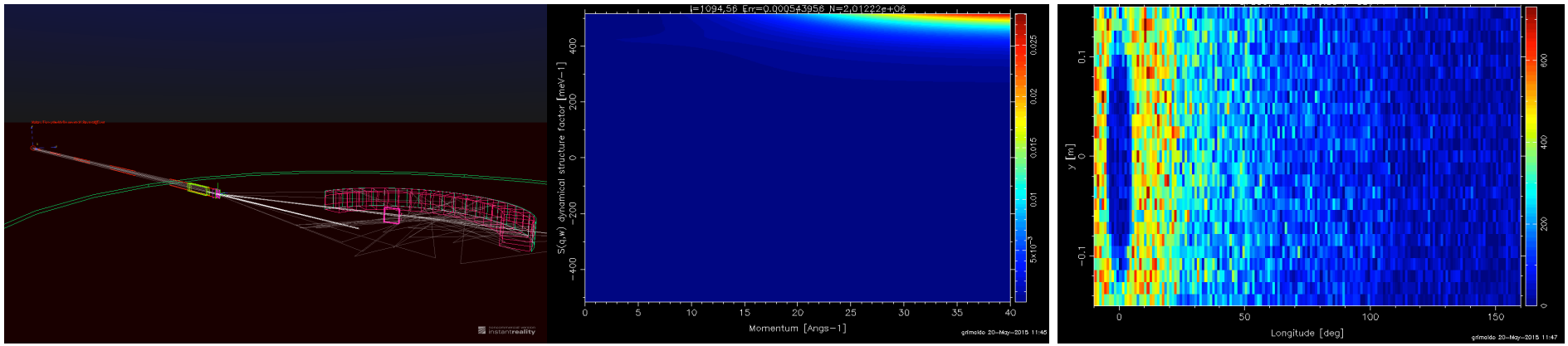
Marco Grimaldo, Diane Lançon

Outline

- What is a virtual experiment?
- Why make it virtual?
- Schematic Neutron-Matter Interaction
- Examples
- Other software

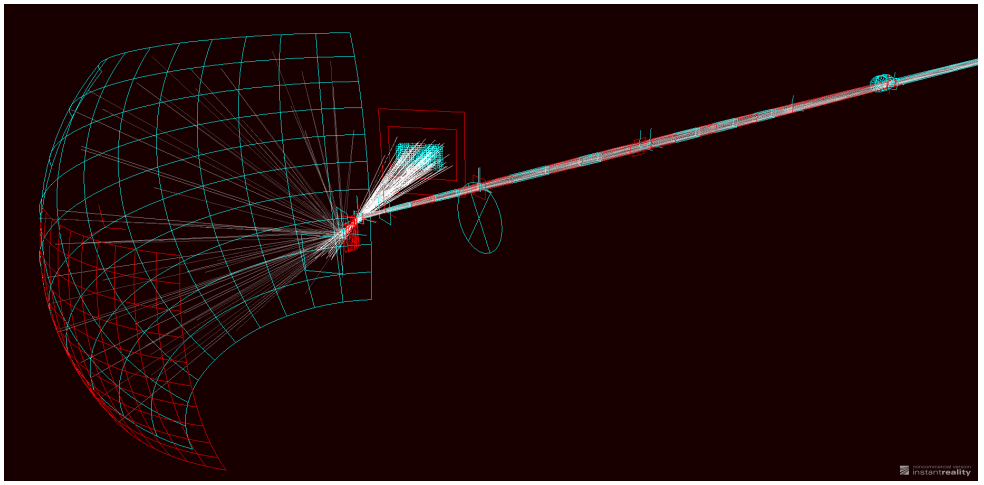
Virtual experiment: what is it?

$$\text{instrument simulation} \otimes S(q,\omega)\ \text{sample} = \text{virtual experiment}$$



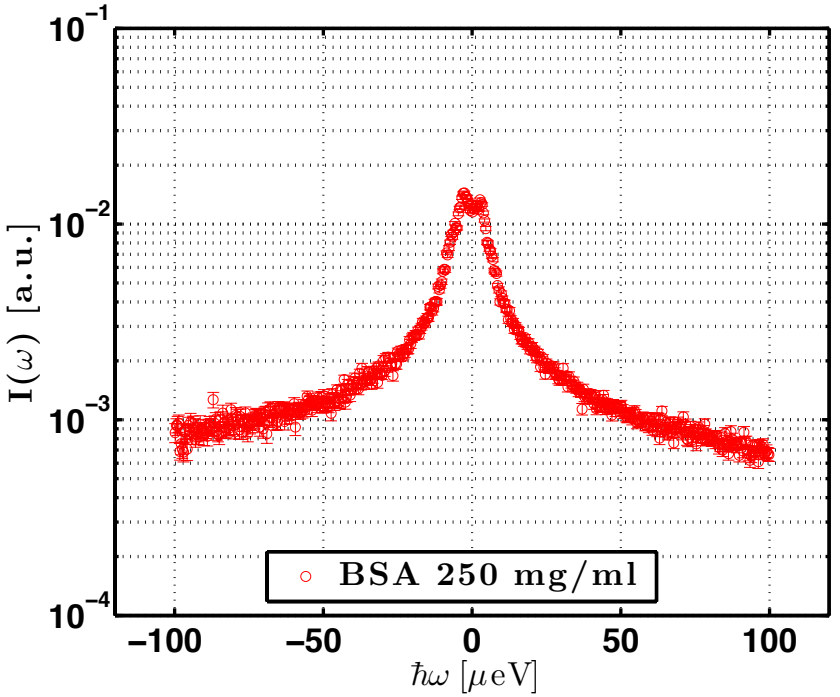
Instrument Simulation
- reminder -

- Monte Carlo simulation
- Neutron rays with weight factors
- Instrument as a sequence of components
  - Sources
  - Moving optics
  - Static optics
  - Detectors



S(q,ω) sample

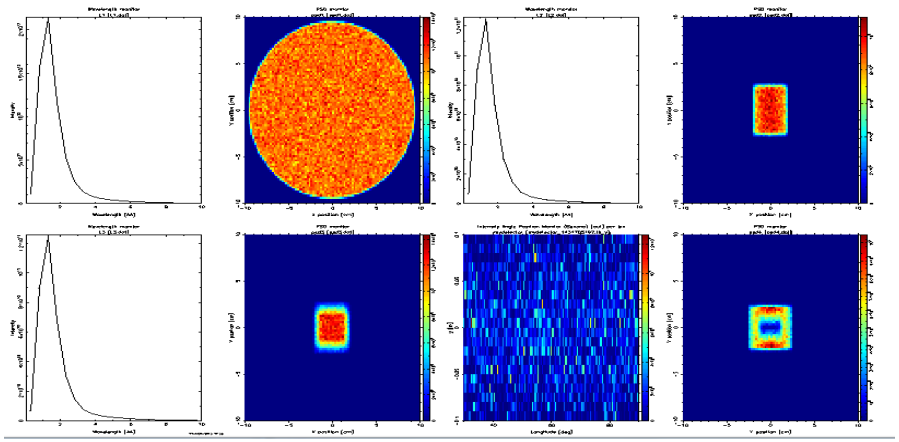
- MD Simulation
- Experiment
- Analytical description



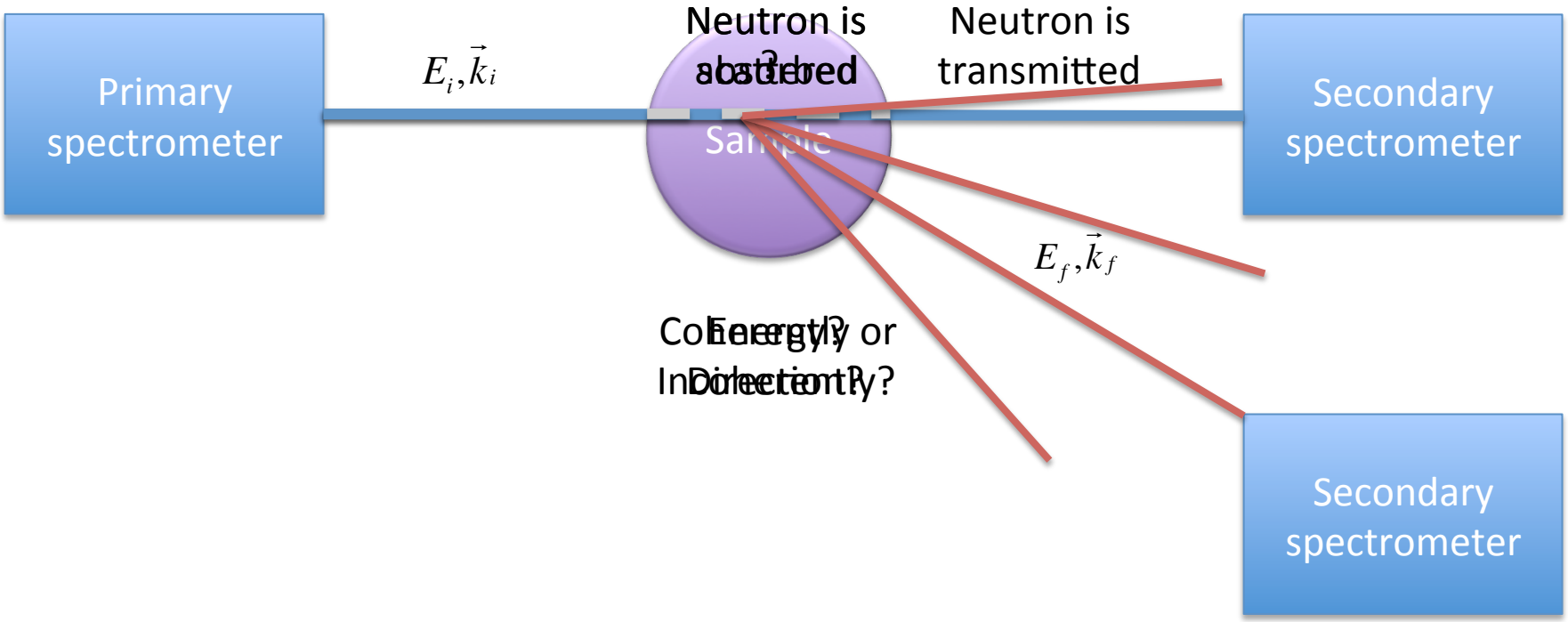
Virtual experiments – Why?

To help with the real experiment

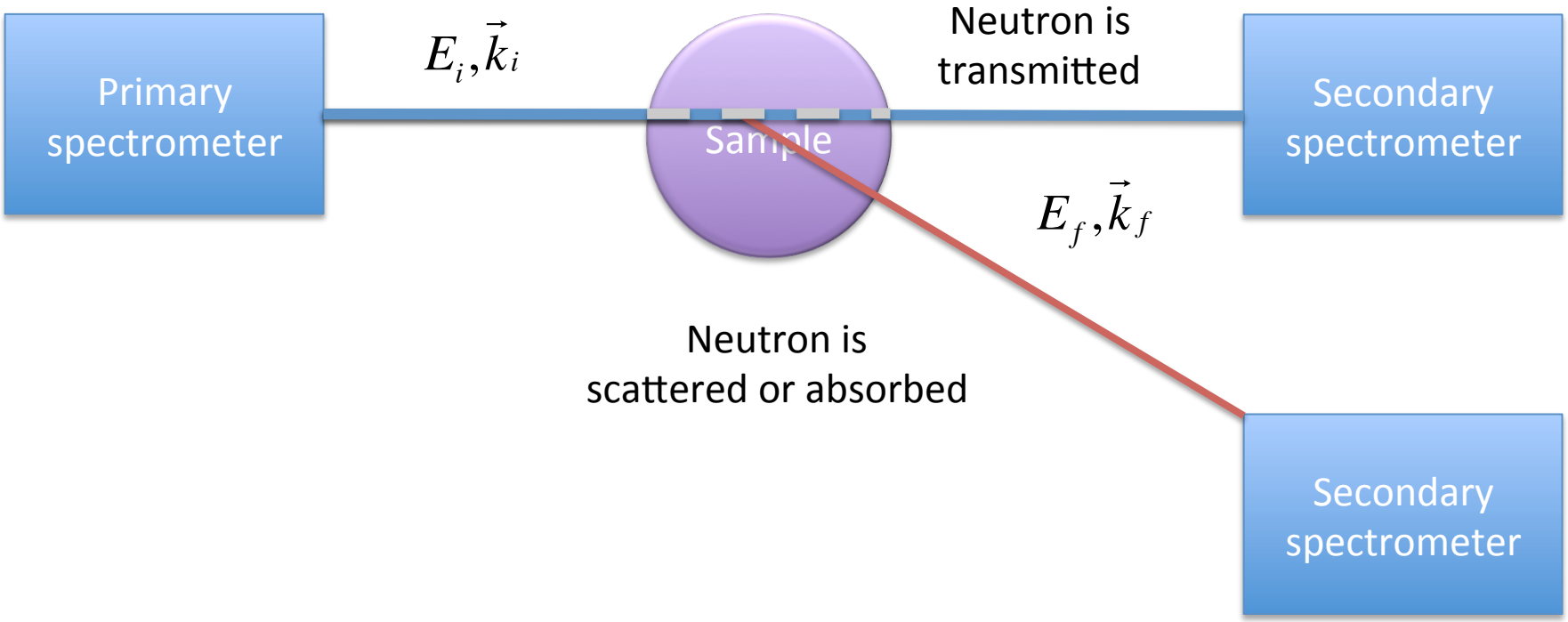
- Training
- Experiment planning
  (e.g. estimating counting time)
- Diagnostics
- Help with experimental data analysis



Schematic neutron-matter interaction



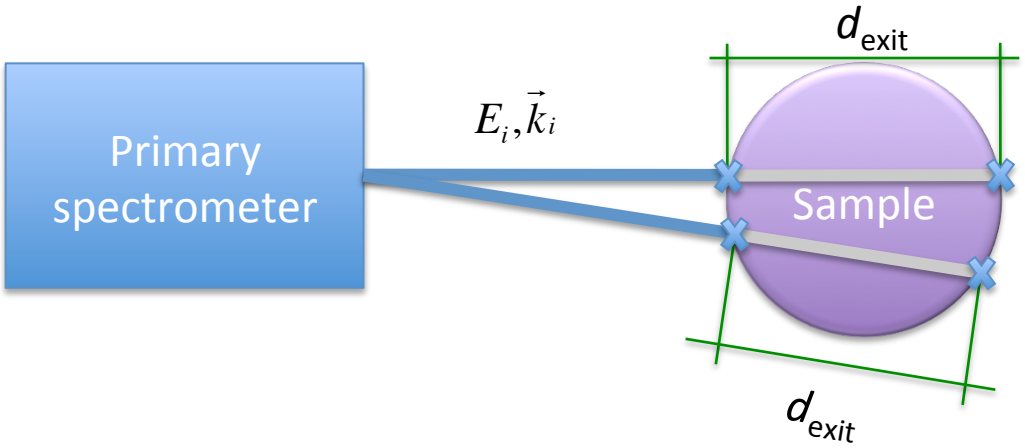
Schematic neutron-matter interaction



Schematic neutron-matter interaction

Will there be an interaction with the sample?

Compute propagation path length in the material



Absorbed? Transmitted? Scattered?

Cross section

Will there be an interaction with the sample?

Evaluate the total cross section $\sigma_{\text{tot}}(E_i) = \sigma_{\text{abs}}(E_i) + \sigma_{\text{s}}(E_i)$

Absorption $\sigma_{\text{abs}}(E_i) = \sigma_{\text{abs}}^{2200} \dfrac{2200}{\sqrt{2E_i / m}}$

Scattering $\sigma_s(E_i) = \int\int \dfrac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E_f} \mathrm{d}\Omega\, \mathrm{d}E_f = N \int\int \sigma S(q,\omega) q \, \mathrm{d}q \, \mathrm{d}\omega$

$\vec{q} = \vec{k}_i - \vec{k}_f$

$\dfrac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\, \mathrm{d}E_f} = \dfrac{\sigma}{4\pi} \dfrac{k_f}{k_i} N S(q,\omega)$

In good approximation $\sigma_s(E_i) \cong \dfrac{N}{2k_i^2} \int_0^{2k_i^2} \sigma S(q) q \; \mathrm{d}q$

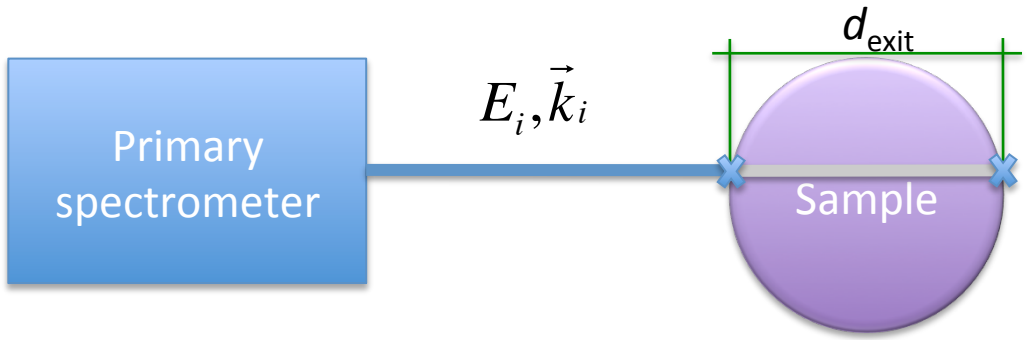
Transmission

Will there be an interaction with the sample?

- In McStas, neutrons are allowed to be transmitted

Linear attenuation $\mu(E_i) = \rho\sigma_{\text{tot}}(E_i)$ Atomic number density ρ

Transmission probability $P_t = \exp(-\mu(E_i)\, d_{\text{exit}})$



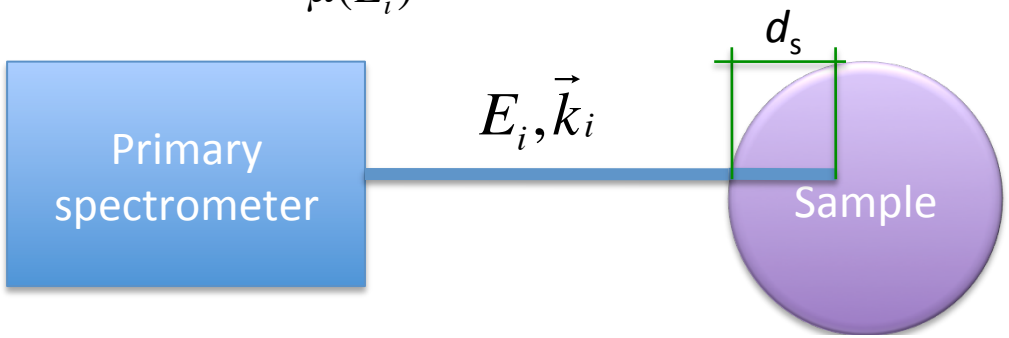
- Random number $\xi_t \in [0,1]$
- If $\xi_t < P_t$ → neutron is transmitted
  Else → neutron is interacting with the sample

Scattering and absorption

Which kind of interaction?

- Either absorbed or scattered
  - Change neutron weight $\pi_1 = \frac{\sigma_s(E_i)}{\sigma_{\text{tot}}(E_i)}$
- Probability coherent scattering $P_{\text{coh}} = \sigma_{\text{coh}}(E_i) / \sigma_s(E_i)$
- Probability incoherent scattering $P_{\text{inc}} = 1 - P_{\text{coh}}$
- Position of scattering along path

$$d_s = -\frac{1}{\mu(E_i)} \ln(1 - \xi_d[1 - \exp(-\mu(E_i) d_{\text{exit}})])$$



Choice of energy transfer

Final state of the neutron?

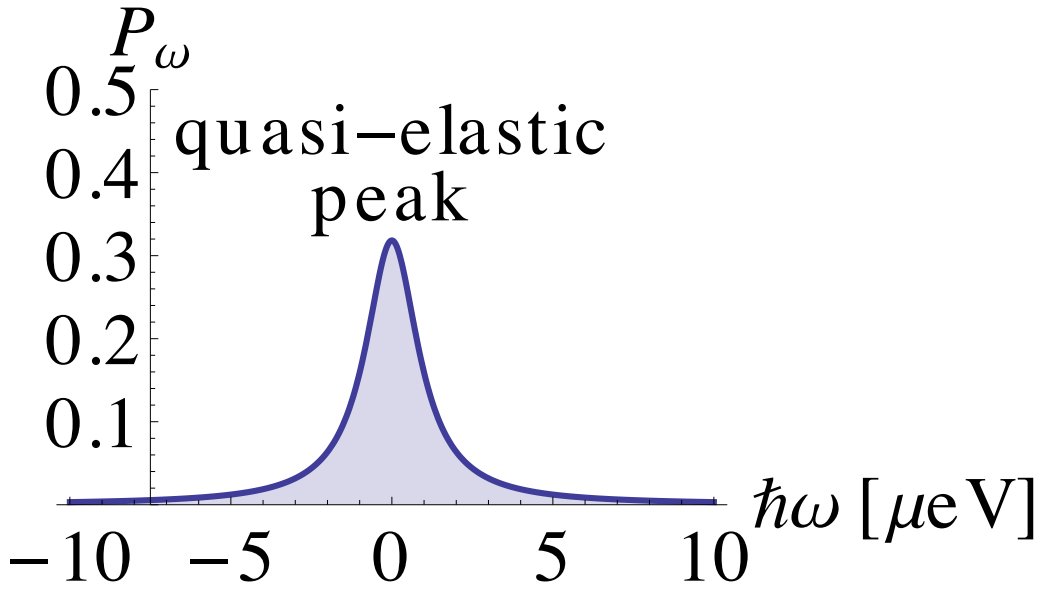
Probability distribution for ω

$$P_\omega(\omega) = \frac{\int_0^{q_{\max}} S(q,\omega)\,\mathrm{d}q}{|S|}$$

$$|S| = \int\int S(q,\omega)\,\mathrm{d}q\,\mathrm{d}\omega$$

Pick random $\xi_\omega \in [0,1]$ and find ω such that

$$\xi_\omega = \int_{\omega_{\min}}^{\omega} P_\omega(\omega')\mathrm{d}\omega'$$



$$S(q,-\omega) = e^{\hbar\omega/k_B T} S(q,\omega)$$

Choice of energy transfer

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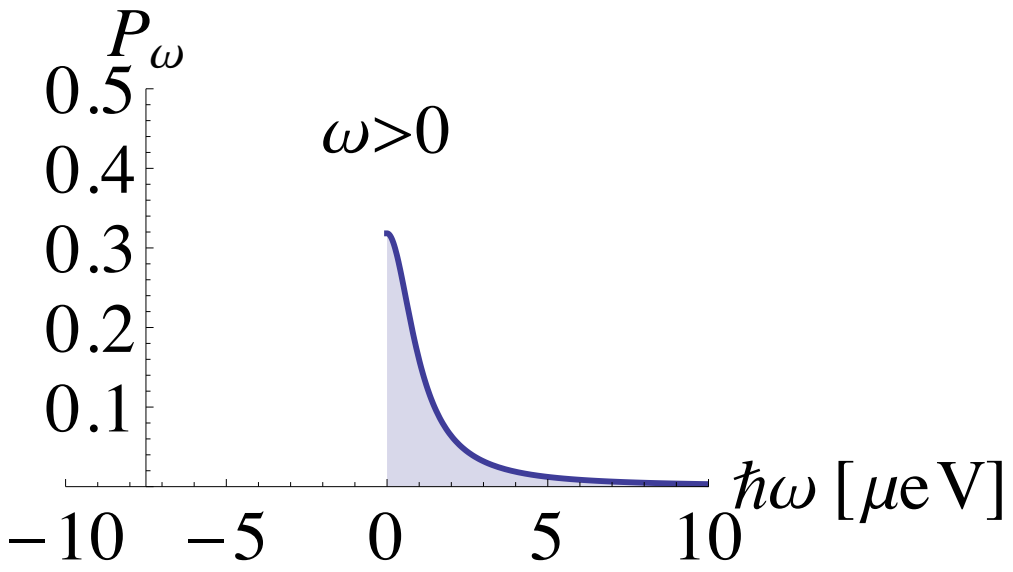

Choice of energy transfer

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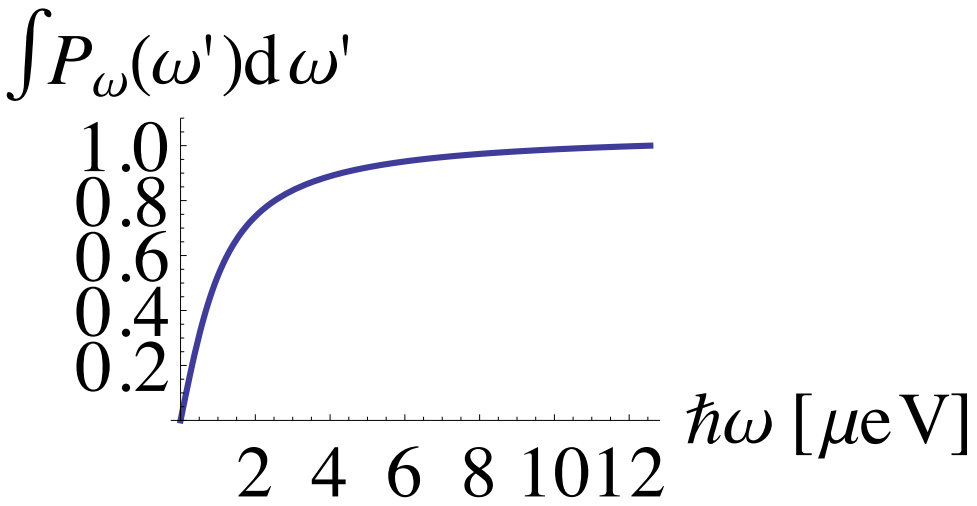

Choice of energy transfer

Final state of the neutron?

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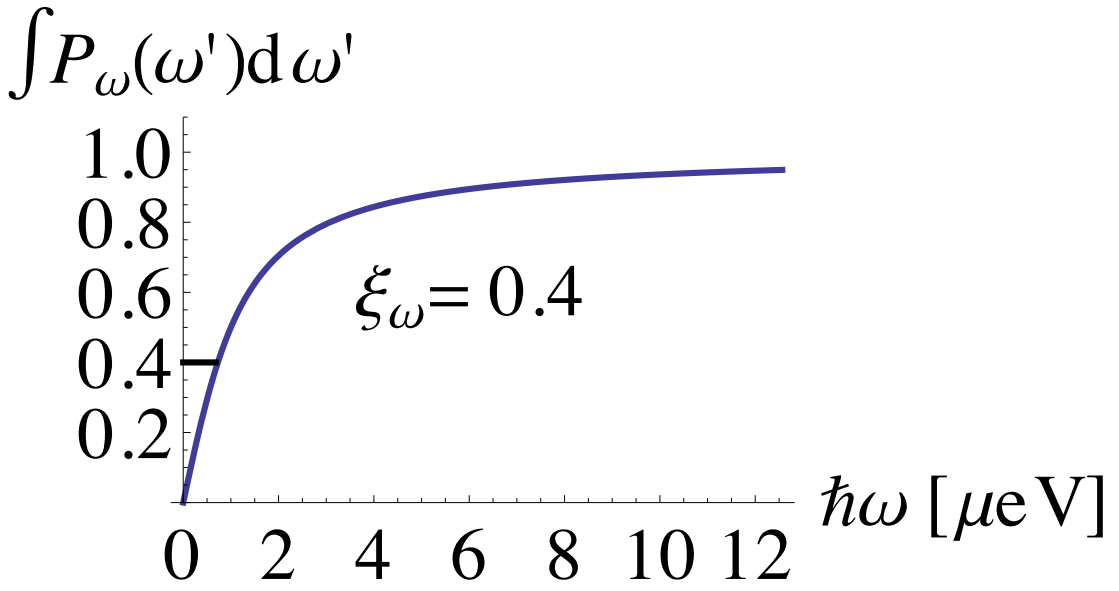


Choice of energy transfer

Final state of the neutron?

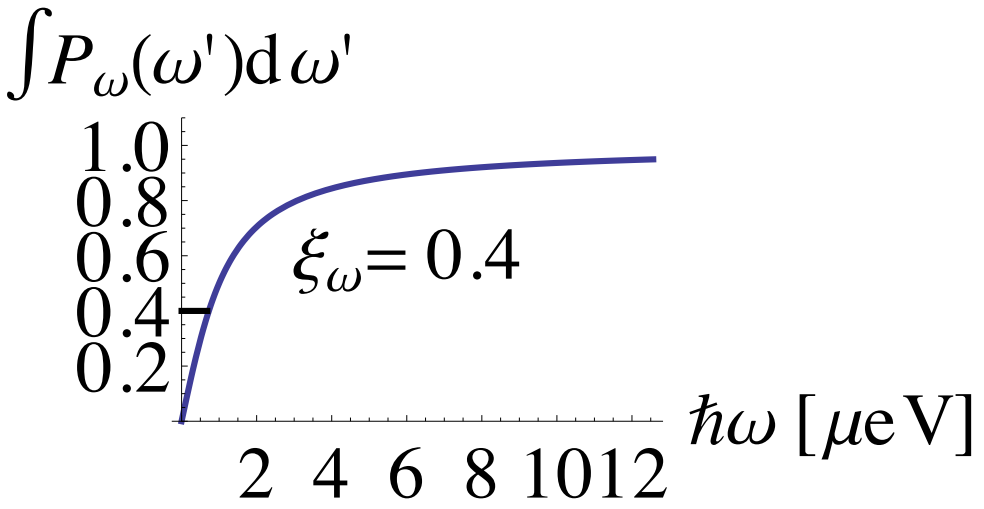
Probability distribution for ω

$$P_\omega(\omega) = \frac{\int_0^{q_{\max}} S(q,\omega)\,\mathrm{d}q}{|S|}$$

$$|S| = \int\int S(q,\omega)\,\mathrm{d}q\,\mathrm{d}\omega$$

Pick random $\xi_\omega \in [0,1]$
and find ω such that

$$\xi_\omega = \int_{\omega_{\min}}^{\omega} P_\omega(\omega')\mathrm{d}\omega'$$



Choice of energy transfer

Final state of the neutron?

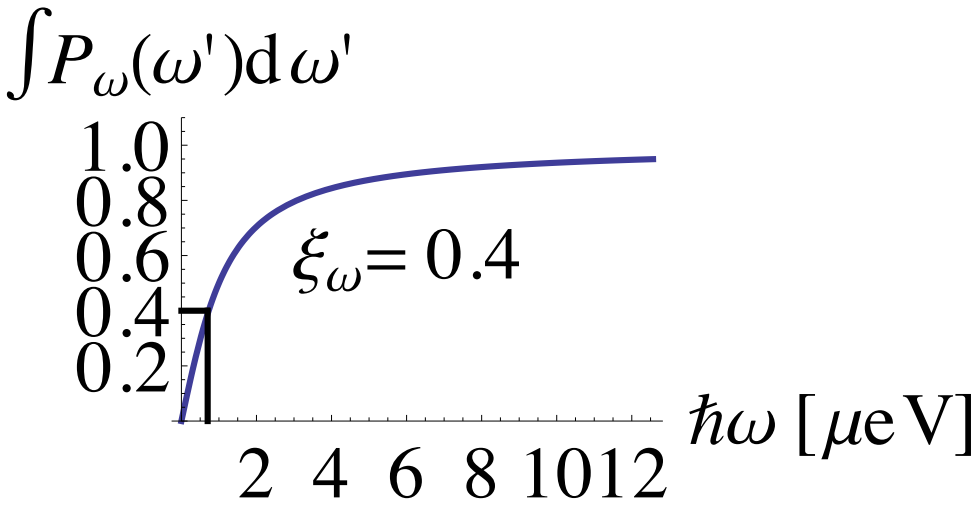
Probability distribution for ω

$$P_\omega(\omega) = \frac{\int_0^{q_{\max}} S(q,\omega)\,\mathrm{d}q}{|S|}$$

$$|S| = \int\int S(q,\omega)\,\mathrm{d}q\,\mathrm{d}\omega$$

Pick random $\xi_\omega \in [0,1]$
and find ω such that

$$\xi_\omega = \int_{\omega_{\min}}^{\omega} P_\omega(\omega')\mathrm{d}\omega'$$



Choice of energy transfer

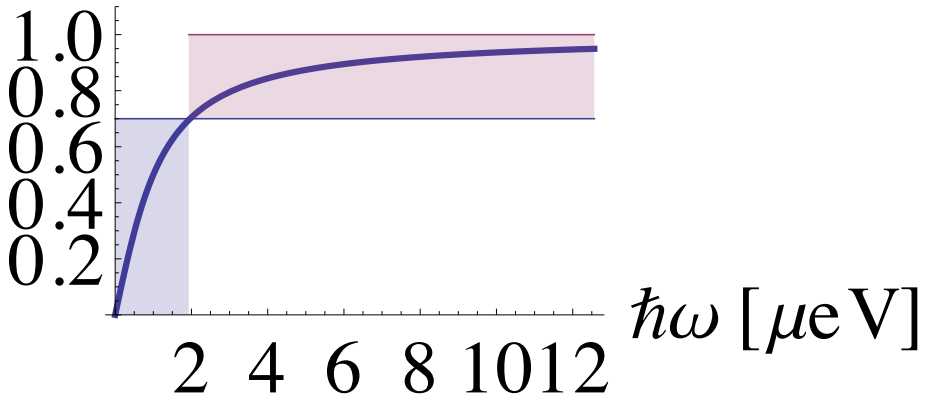
Final state of the neutron?

$$P_\omega(\omega) = \frac{\int_0^{q_{\max}} S(q,\omega)\,\mathrm{d}q}{|S|}$$

$$|S| = \int\int S(q,\omega)\,\mathrm{d}q\,\mathrm{d}\omega$$

$$\xi_\omega = \int_{\omega_{\min}}^{\omega} P_\omega(\omega')\mathrm{d}\omega'$$

$$\int P_\omega(\omega')\mathrm{d}\omega'$$



Choice of momentum transfer

Final state of the neutron?

- Probability distribution for q, given ω (from previous step)

$$P_q(q \mid \omega) = \frac{S(q,\omega)}{S(q)}$$

- Pick a random $\xi_q \in [0,1]$ and find q such that

$$\xi_q = \int_{q_{\min}}^{q} P_q(q' \mid \omega)\,\mathrm{d}q'$$

Solving selection rules

Final state of the neutron?

- Energy and momentum transfer must satisfy

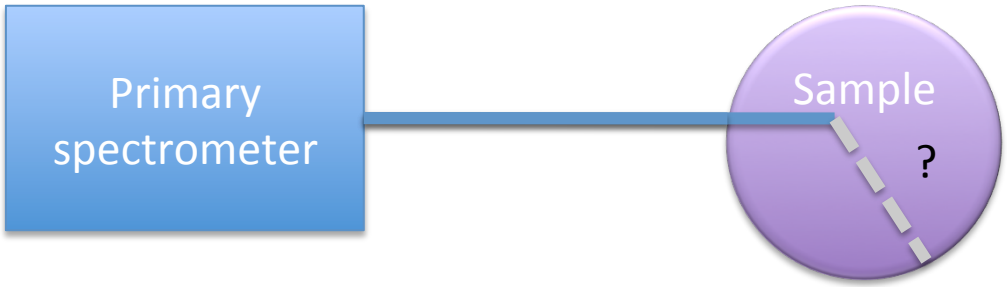
$$\hbar\omega = E_i - E_f = \frac{\hbar^2}{2m}(k_i^2 - k_f^2)$$

$$\vec{q} = \vec{k_i} - \vec{k_f}$$

- If not possible with chosen ω and q, choose new ones

Iteration

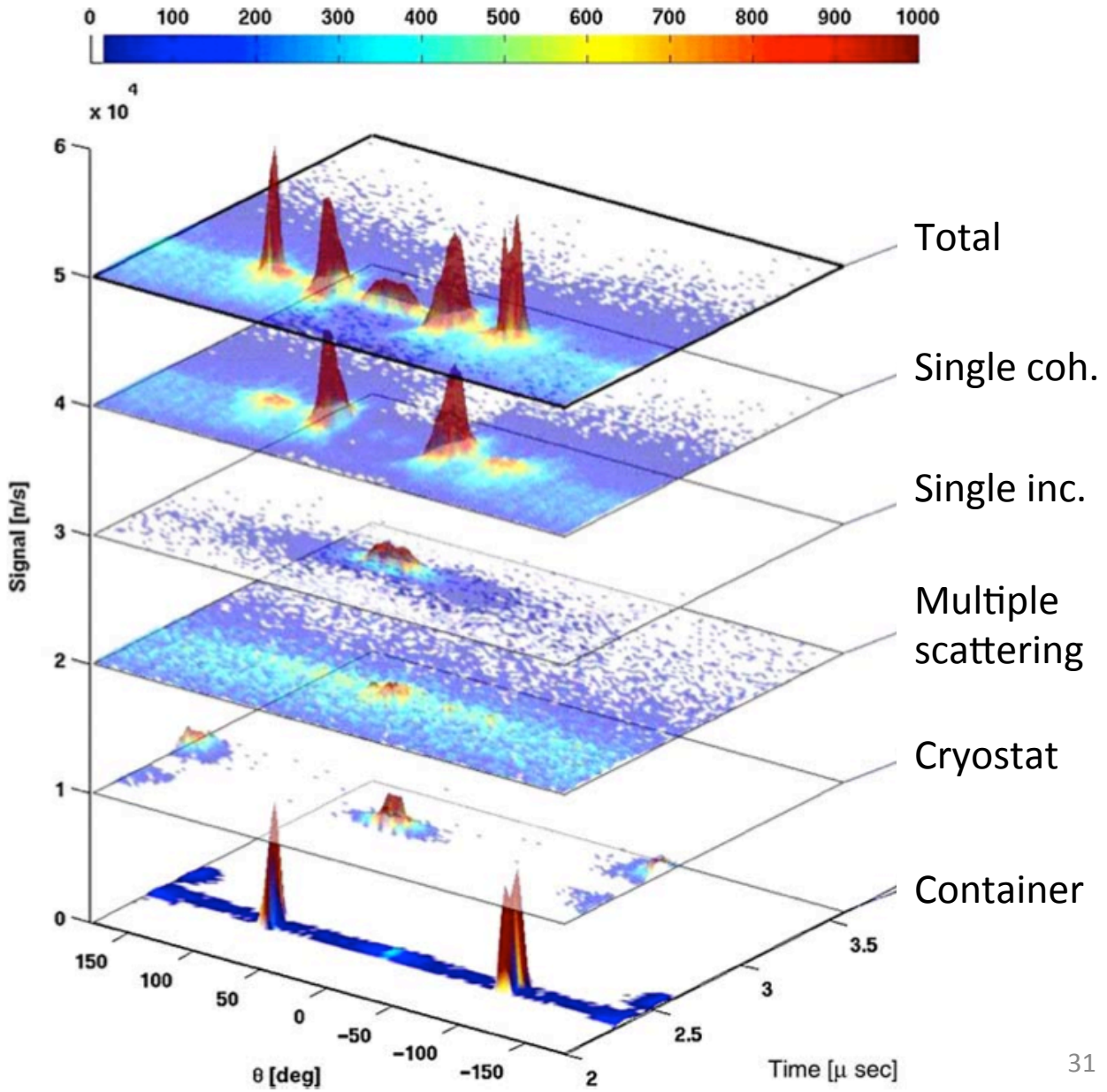
Repeat all the steps until the neutron is out of the sample



Then, neutrons may interact with other components in the secondary spectrometer

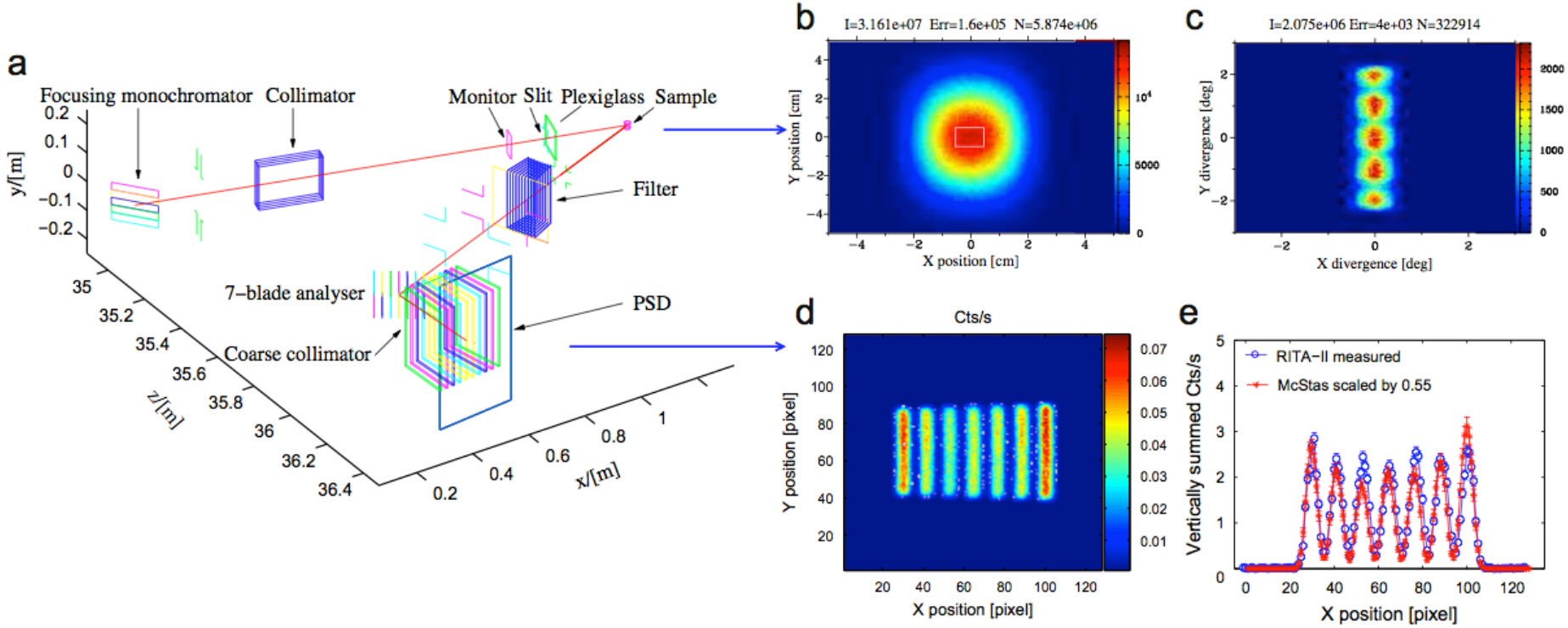
Example 1 - Virtual Experiment on IN6

Separation of different **contributions** to total scattering



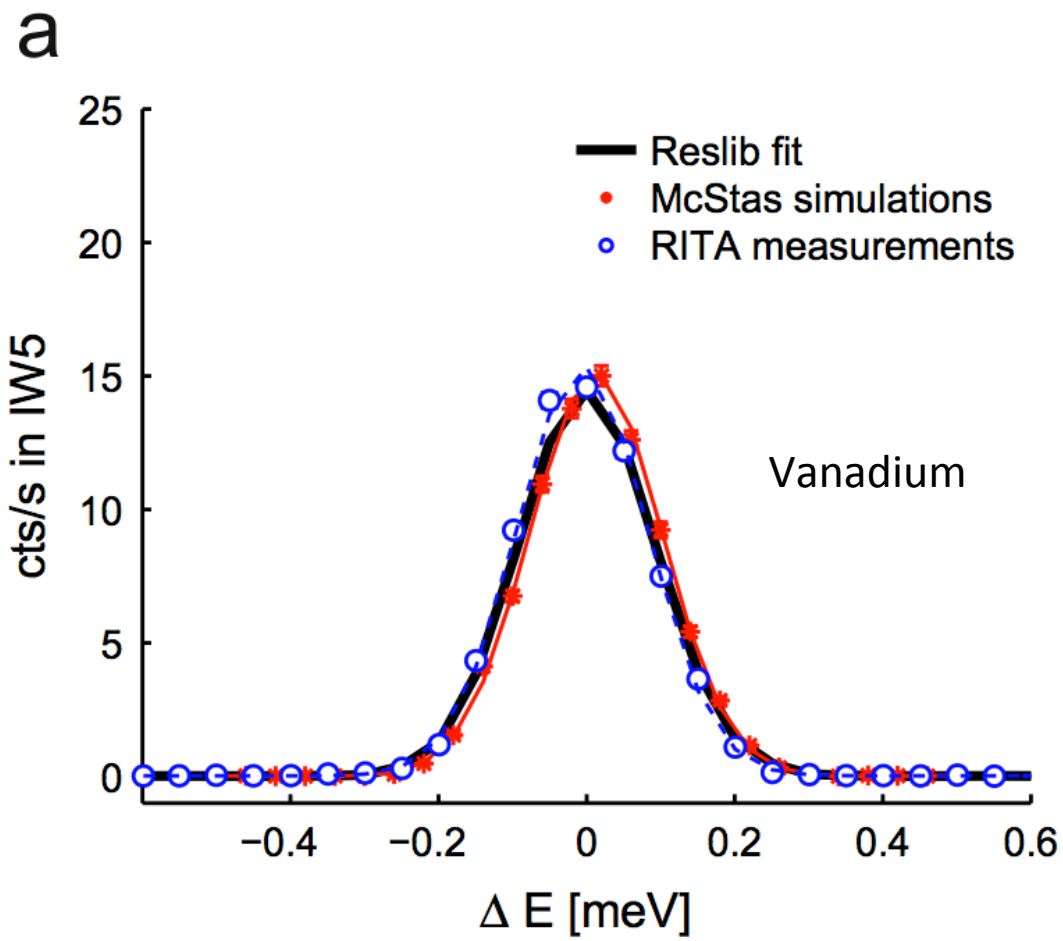
Example 2 - Virtual Experiment on RITA-II

Triple-axis spectrometer at PSI (Switzerland)
- Vanadium



Example 2 - Virtual Experiment on RITA-II

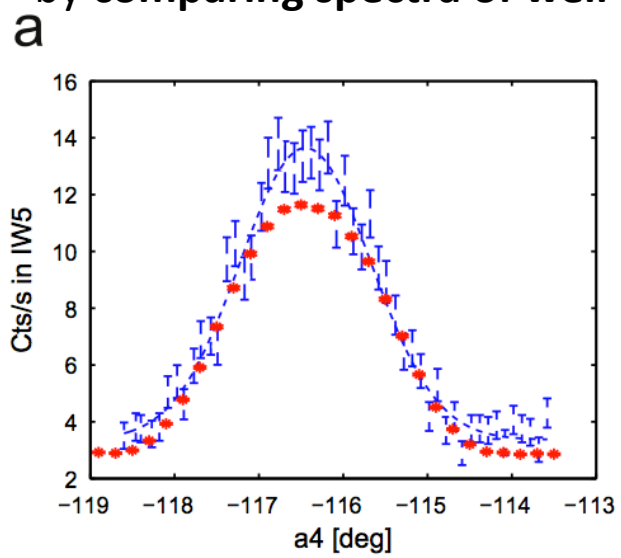
1) Check that the **experimental data** is well reproduced by the virtual experiment by **comparing spectra of well known samples**

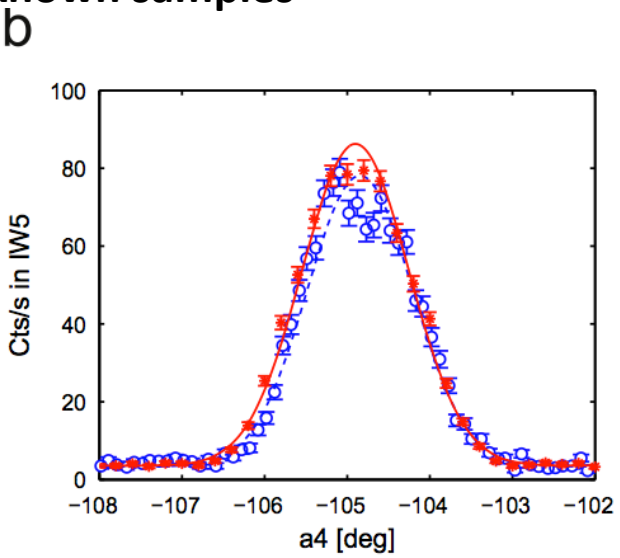


Agreement within 3%

Example 2 - Virtual Experiment on RITA-II

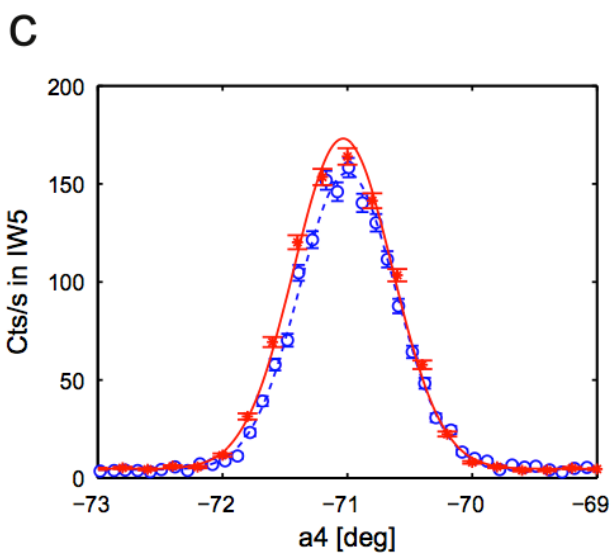
1) Check that the **experimental data** is well reproduced by the virtual experiment by **comparing spectra of well known samples**

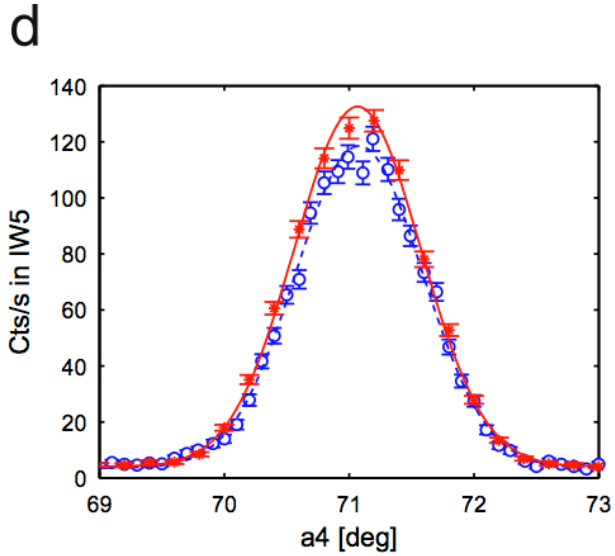




Al_2O_3

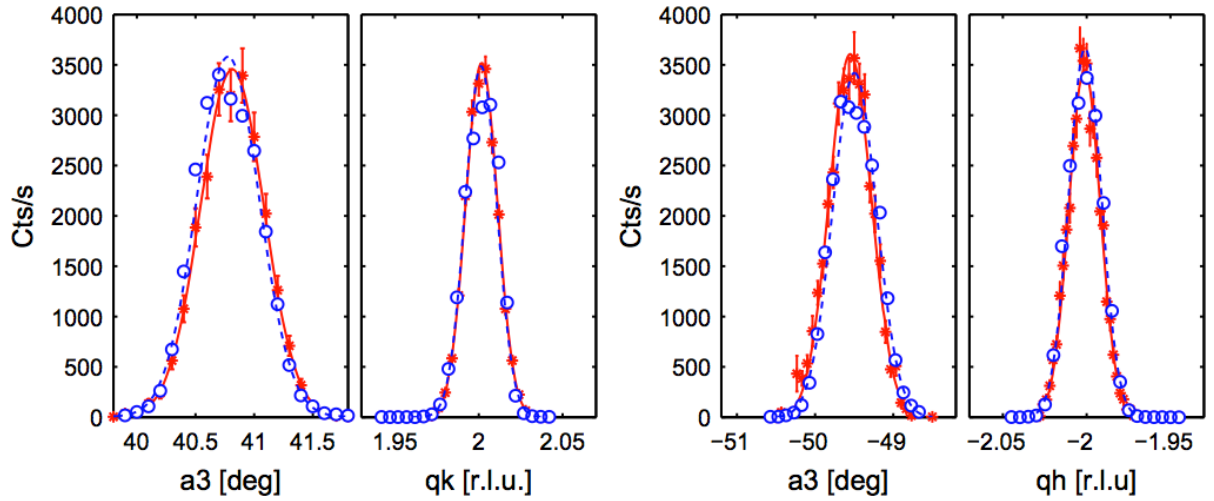
Linewidth agrees within 2%



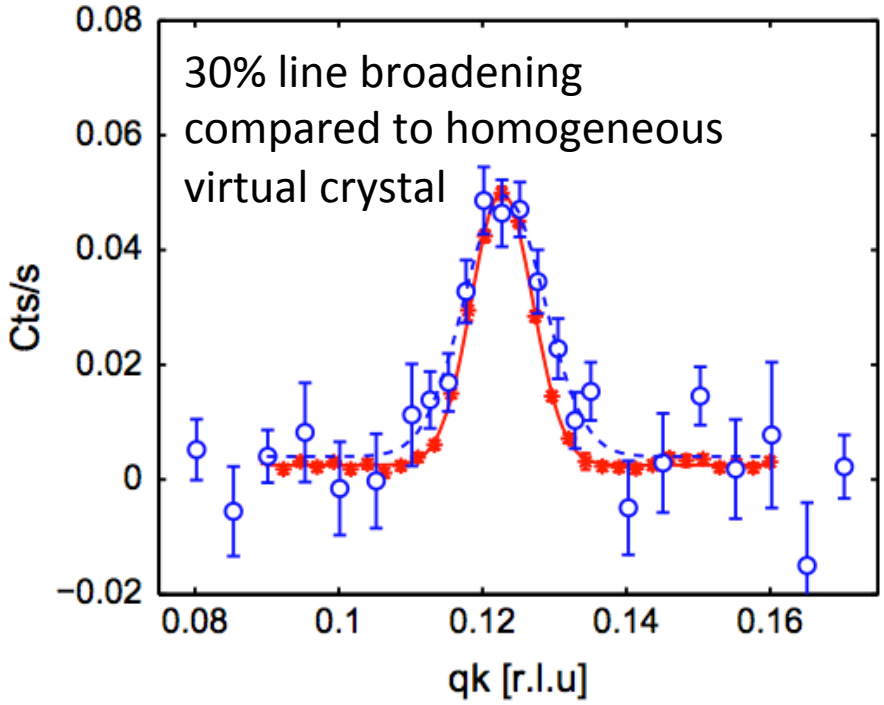


Example 2 - Virtual Experiment on RITA-II

2) Compare **model** in virtual experiment with **experimental data**



LSCO+O x=0.09



Other available software (non exhaustive list)

- Restrax – MC/Analytical mostly TAS
- Simres – Similar to Restrax, less specialized
- MCNP – MC neutron/photon/electron transport
- Vitess – MC neutron instruments, ESS
- NISP – MC neutron instruments, Los Alamos
- guide_bot – beam guide design, writes McStas file
- …

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- McStas manual http://www.mcstas.org/documentation/manual/
- McStas components manual http://www.mcstas.org/download/components/