Design of Neutron Instrumentation *via* Simulation

E. Farhi,
Institut Laue-Langevin, Grenoble, France.

<www.mcstas.org> project supported by EU FP4/5/6/7 since 1996

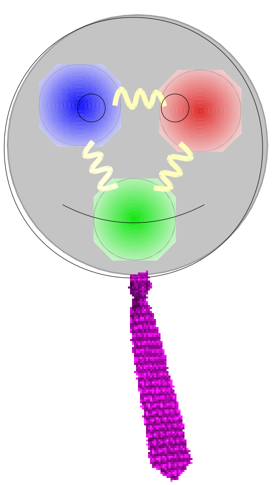
Introducing the Neutron

Electrically Neutral
penetrate deeply into matter – non destructive ;
can not be handled with E/B fields.

Microscopically Magnetic (polarized neutron beams)
they possess a magnetic dipole moment ;
spin is sensitive to B fields, thus can do NMR-like studies.

Ångstrom wavelengths
neutron wavelengths range from 0.1 Å to 1000 Å ;
well suited for studying atomic/molecular structure.

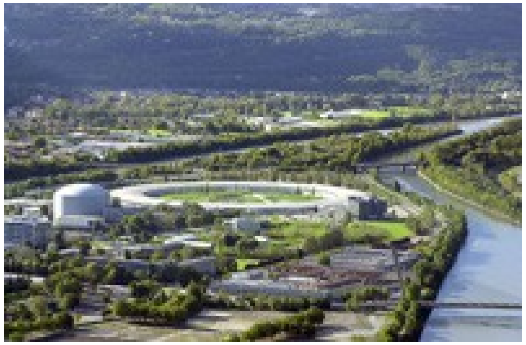
Energies of milli-electronvolts (1 μeV - 1eV)
same magnitude as most motions in solids and liquids ;
suited to studying phonons and magnons.



A fancy neutron

Randomly sensitive (cross sections)
well suited to distinguish light atoms (CNOH) and isotopes within materials.

Usage of neutrons: instruments for users

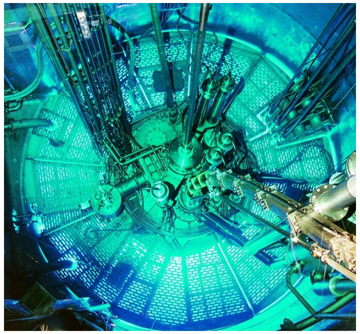


About 5000 users in Europe

in Physics, Chemistry, Biology, and Nuclear Physics

14 neutron facilities – 250 instruments in Europe

within which ILL (started 1971) is the world's most intense.
Neutrons generated in nuclear reactors (ILL, Munich, LLB)
and spallation sources (accelerator based, ISIS, PSI)



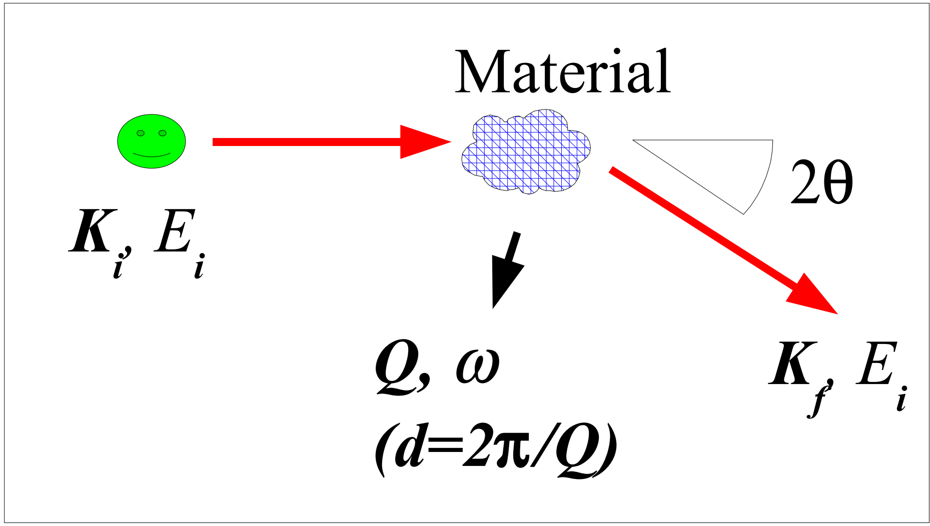
Complementary with X-rays

not sensitive to the same features, but same wavelength range

Used to measure structure and dynamics of materials

- diffractometers (powders, liquids, crystals) - *structure*
- inelastic scattering spectrometers (powders, liquids, crystals) - *dynamics*
- small angle machines for large scale structures (polymers, colloids, gels)
- magnetic materials structure and dynamics using polarized neutrons (spin)
- nuclear and fundamental physics with neutrons (fission, neutron properties, γ)

Neutrons interact with matter ...



Selections rules

$$K_f = K_i + Q$$
$$E_f = E_i + \omega$$

Bragg's law (diffraction on structure – atoms separated by distance *d*)

$$\lambda = 2\pi / K_i = 2 d \sin\theta$$

Scattering law (intensity per solid angle and energy, dynamics)

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \frac{\sigma}{4\pi} \frac{K_f}{K_i} S(Q,\omega)$$

Dynamical structure factor *$S(Q,\omega)$* is characteristic for each material

Reflects ordering of matter (atom/molecule positions – movements - domains)

Interaction processes

Elastic scattering: no energy exchange with matter

$\omega = 0$, $|Ki|=|Kf|$

Ruled by the Bragg's law → structure $S(Q)=\int S(Q,\omega)\,d\omega$

Inelastic scattering: energy exchange with matter

Neutron can gain or loose energy with is transfered to matter

Couples e.g. to matter dynamics (phonons, magnons, …)

Coherent scattering: atoms/molecules in matter vibrates coherently

e.g. Structure (elastic), sound waves, spin waves, ...

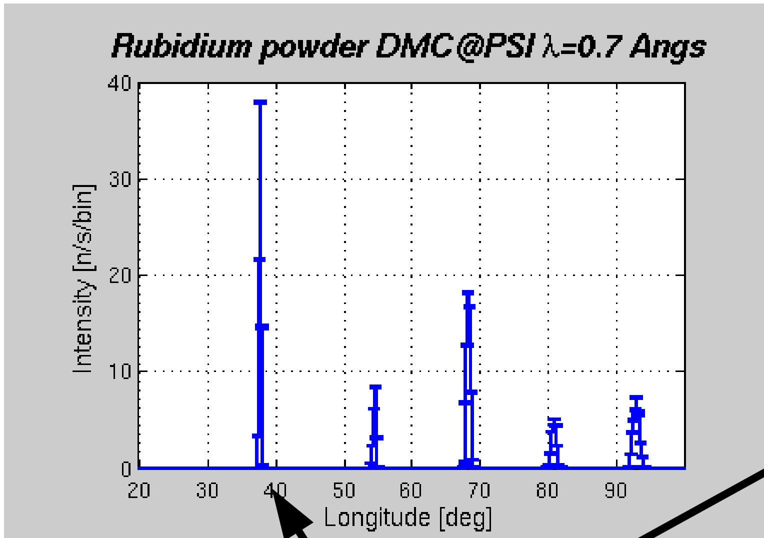
Incoherent scattering: atoms/molecules have random processes in matter.

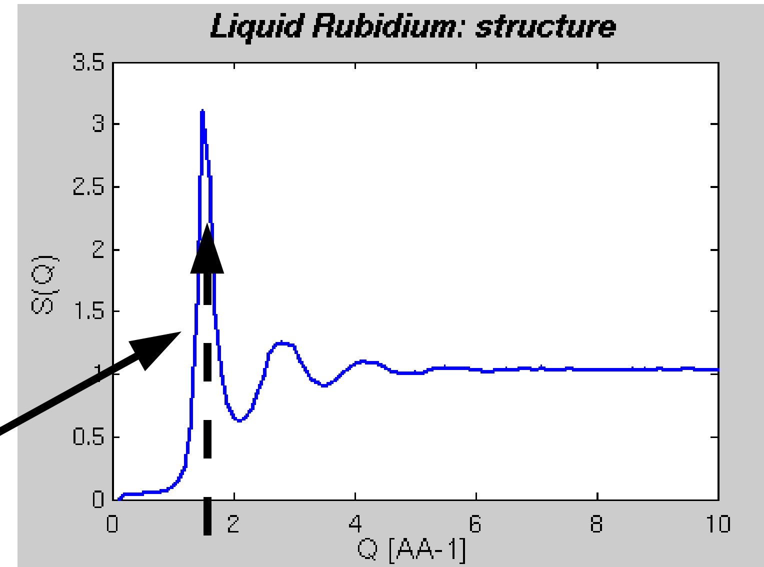
e.g. Isotopes, defects, heat diffusion, ...

Example of materials: powder and liquid

Structure
S(Q)

Elastic scattering
(diffractometer)



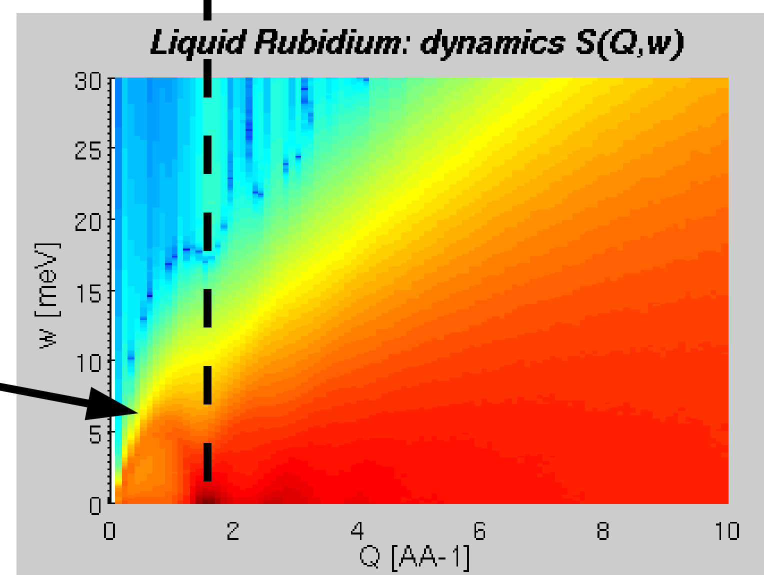


Structure peaks
(atom/molecule spacing)

Dynamics
S(Q,ω)

Inelastic scattering
(time-of-flight)

Phonons
(atom/molecule motions)



Why simulate neutron instruments ?

Help instrument responsibles

- instrument optimization and design

Help scientists

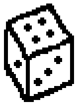
- plan experiments (for proposal application: *is the experiment feasible ?*)
- guide experiments (during beam time allocation: *optimize beam usage*)
- help understand results and analyze data (after experiment: *what is <u>this</u> ?*)

How to proceed ?

- Install a Monte Carlo simulation software for neutron instrumentation simulation: ***McStas***, VitESS, NISP, ResTrax
- Collect information about instrument geometry and configuration
- Collect information about the sample/measurement to be performed
- Use existing instrument model/template and customize it or write model from scratch
- Launch simulation
- Compare with what you (think) know/measure

Flexible, general simulation utility for neutron scattering experiments.

Original design for *M*onte *C*arlo *S*imulation of *t*riple *a*xis *s*pectrometers.



Developed at RISØ and ILL (started 1998).
Mainly funded by EU (FP 4-7): 2.5+1 people full time, plus projects.
Open source, GPL2. Works on all systems, binaries for *Linux, Win$, MacOSX*

Most widely used code in its ecological niche (compared to other similar codes)..

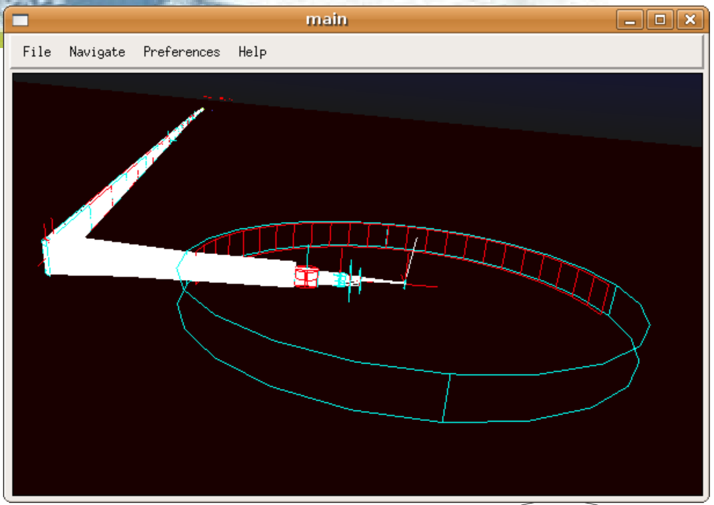
Probably a few hundred users worldwide (160 registered)
some contributors (community based).
Has been used to model most existing and future neutron scattering instruments.

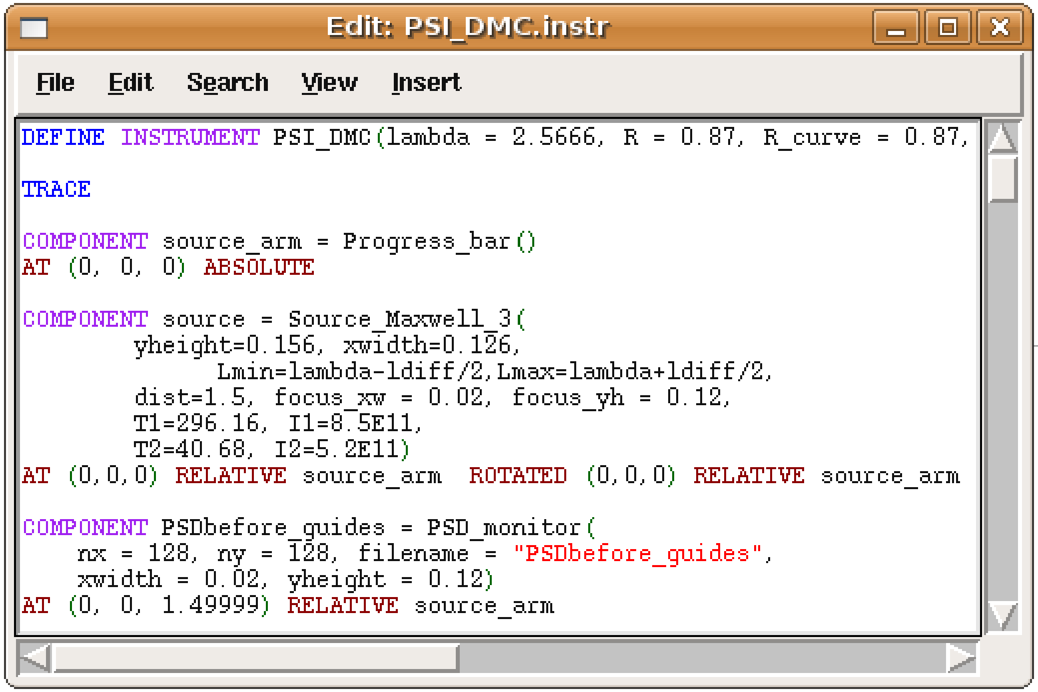
<www.mcstas.org>

mcstas-users@mcstas.org *mailing list*
mcstas-support@mcstas.org *developer contact*

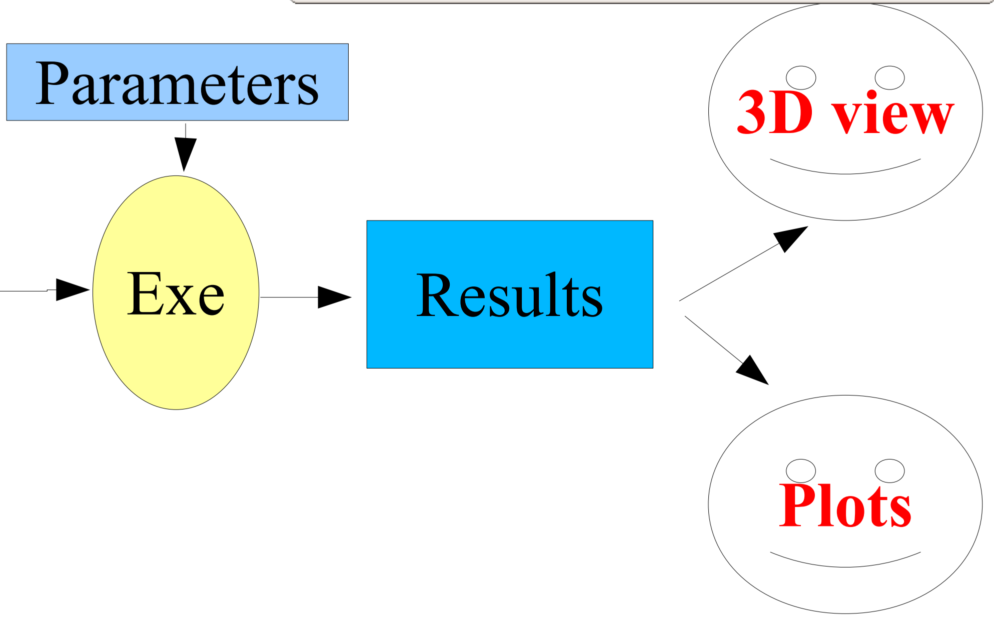
Main capabilities of *McStas*

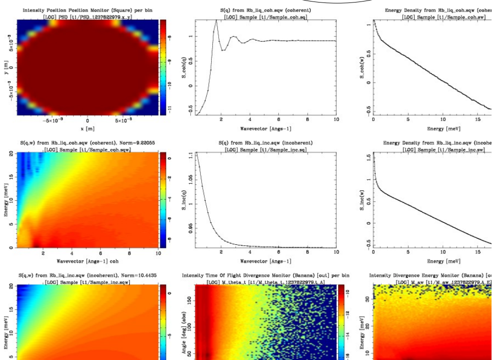
McStas requires an instrument description (text)
Many instrument examples are given with the software, covering all instrument classes (TOF, TAS, SANS, DIF, ...).






```
DEFINE INSTRUMENT PSI_DMC(lambda = 2.5666, R = 0.87, R_curve = 0.87,

TRACE

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

COMPONENT source = Source_Maxwell_3(
        yheight=0.156, xwidth=0.126,
              Lmin=lambda-ldiff/2,Lmax=lambda+ldiff/2,
        dist=1.5, focus_xw = 0.02, focus_yh = 0.12,
        T1=296.16, I1=8.5E11,
        T2=40.68, I2=5.2E11)
AT (0,0,0) RELATIVE source_arm  ROTATED (0,0,0) RELATIVE source_arm

COMPONENT PSDbefore_guides = PSD_monitor(
    nx = 128, ny = 128, filename = "PSDbefore_guides",
    xwidth = 0.02, yheight = 0.12)
AT (0, 0, 1.49999) RELATIVE source_arm
```





McStas creates an instrument executable model for which configuration parameters can be changed at will.

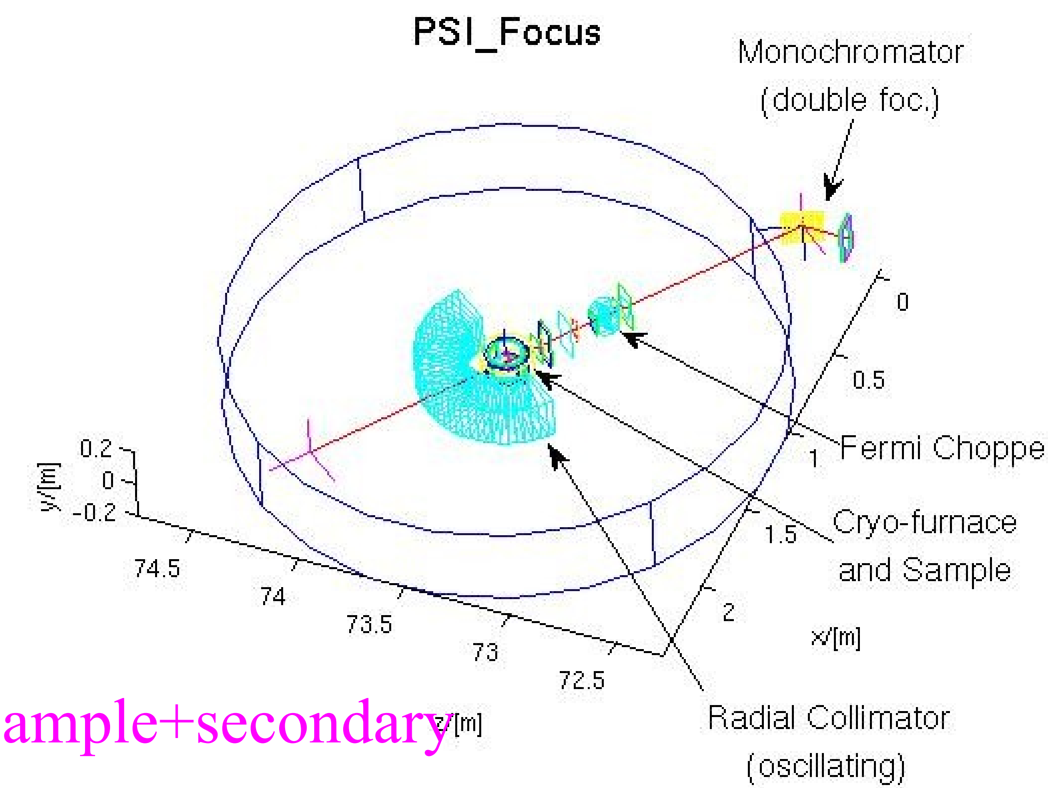
More about *McStas*

McStas is a compiler. It translates a clean instrument description (using a dedicated grammar) into a flat C file, which is compiled and executed.
Components used instruments are pieces of C code, with dedicated grammar and function calls to ease programming.
Creating new instruments and components is *damn* easy.

Documentation:

- Extensive code documentation
- User and Component manuals,
- mailing list/forum, tutorial,
- 50 instrument examples.

McStas has built-in support for cluster and grid computing.



Simulation = Source+guide+primary+sample+secondary

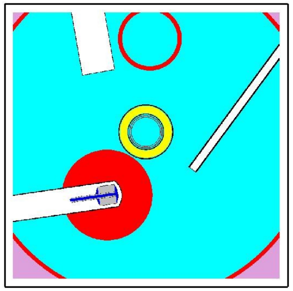
Source: Generating neutron events

Neutron events may be currently generated from:

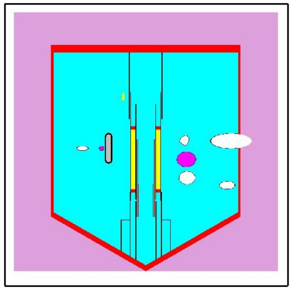
- A black body (Maxwellian distributions)
- Measured flux/divergence distributions
- MCNP and Tripoli (nuclear reactor simulation codes) event files

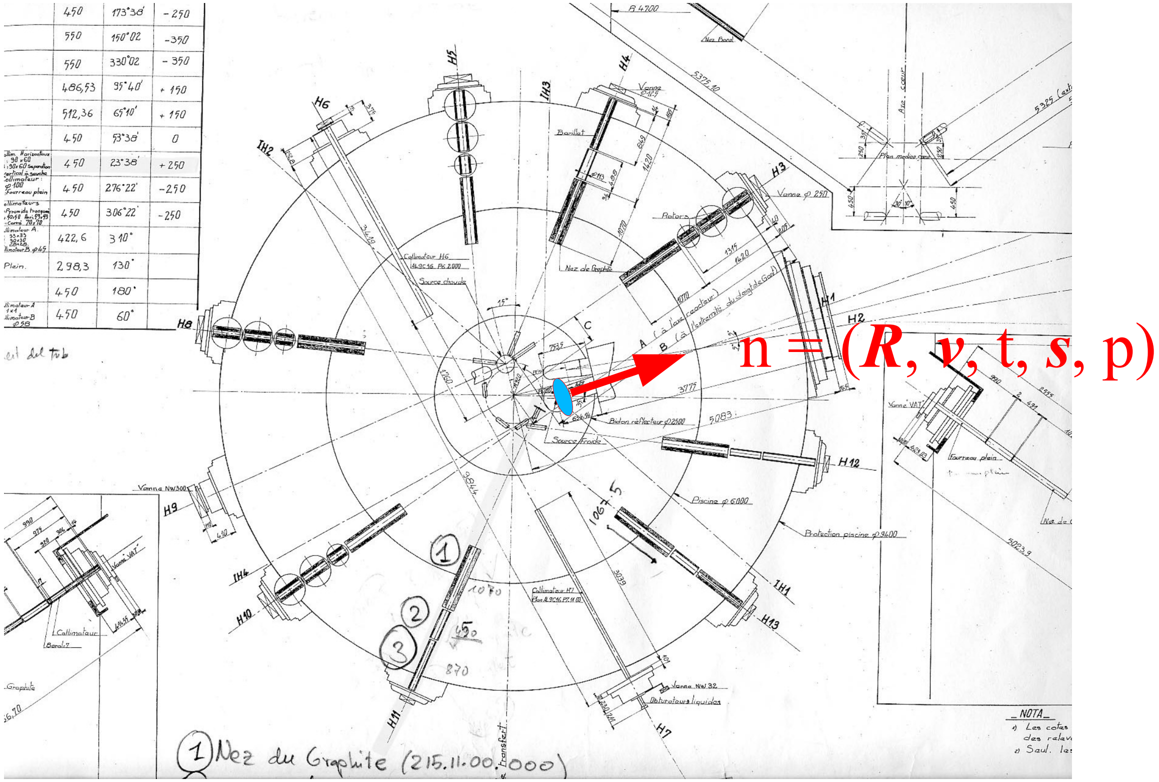
Other neutron generators are in principle easy to write (e.g. from GEANT, FLUKA, ...)

top



side



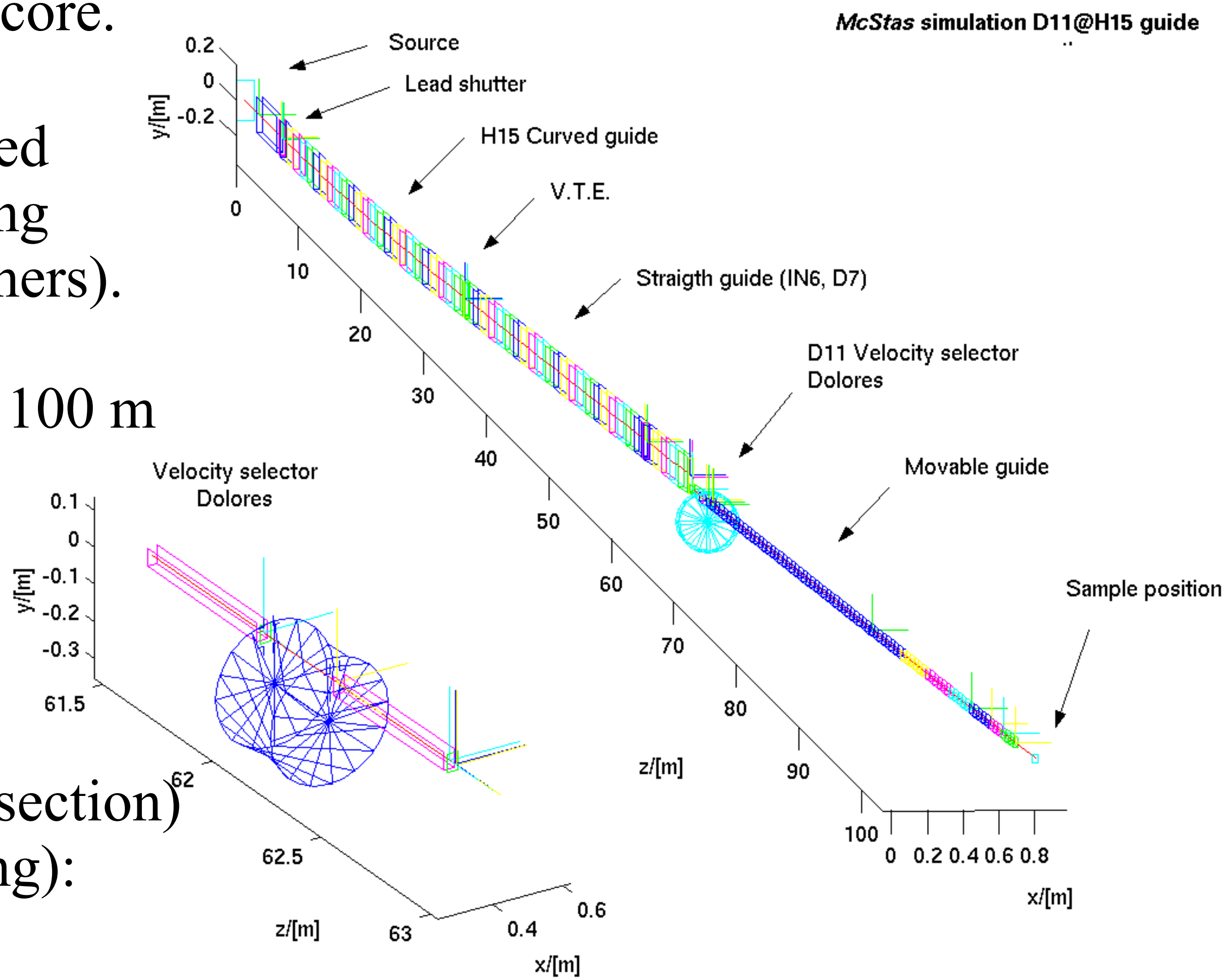


Guide systems: bring neutrons to instruments

Guide systems are usually curved to remove γ rays from the core.

Here is a 3D view generated from the H15 guide, feeding the D11 instrument (polymers).

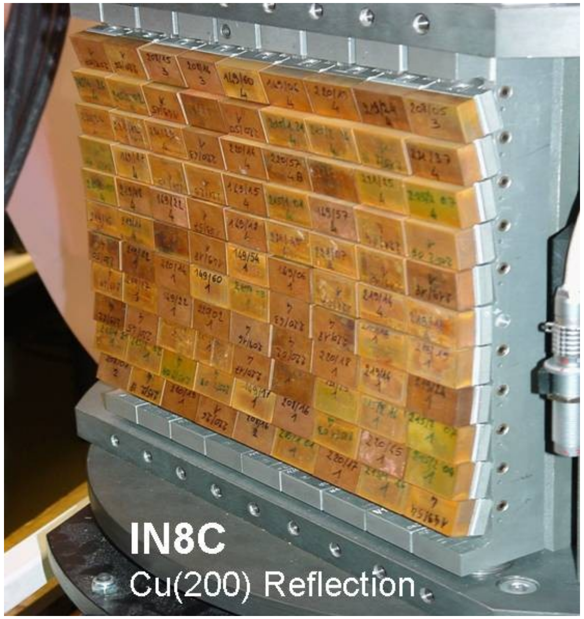
Sections: 3x20 cm, length 100 m



Optimize:

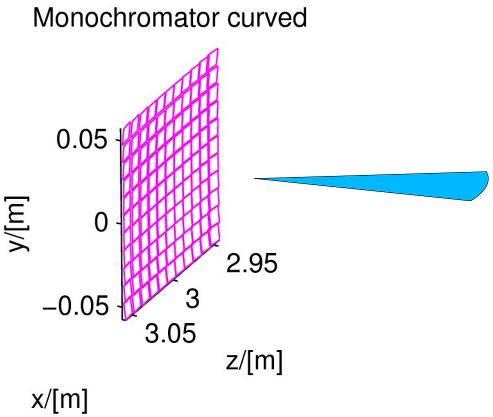
- Guide shape (curvature, section)
- Guide reflectivity (coating):
  Ni, Ti
  R=1 for $\alpha \sim 0.1\ \lambda$

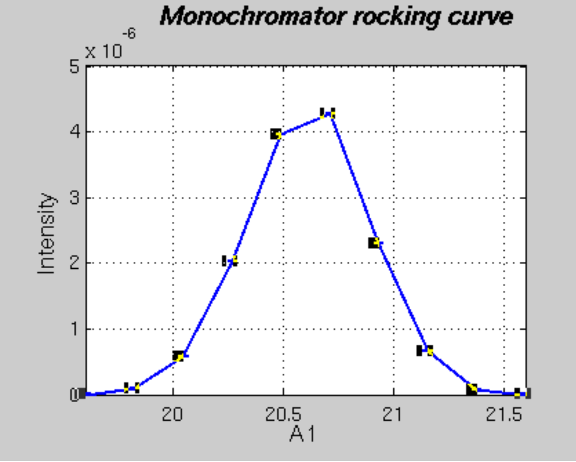
Neutron optics: monochromators (primary spect.)



Monochromators are used to extract a sharp neutron energy distribution from a white beam. Rely on Bragg's law.

Use single crystal assembly, with focusing geometry.
Size: Typically 20x20 cm



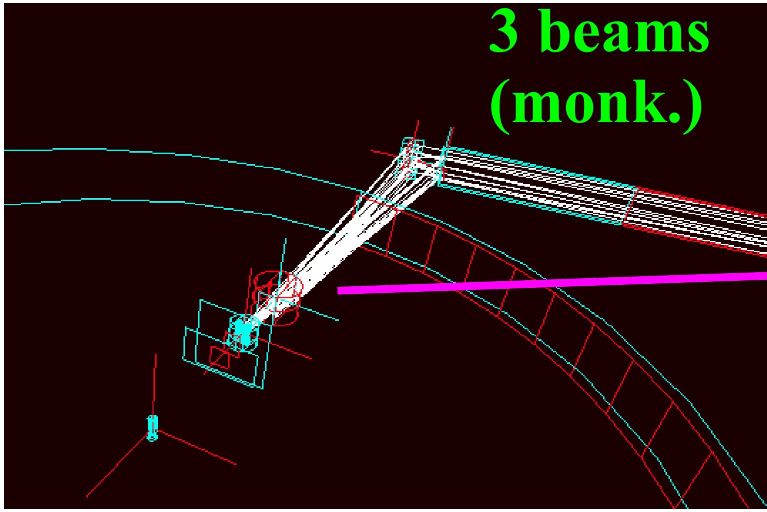


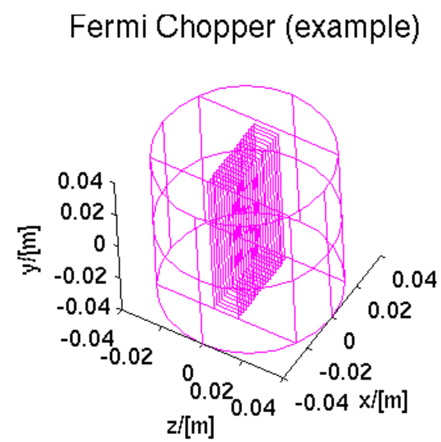
Cu, Ge, Si, C (graphite)
CuMnAl, CoFe (pol.)

Design and characterisation are eased using simulation,

- intensity *vs.* curvature radius,
- thickness of blades
- rocking curve (reflectivity)
- scattering from the mechanics (generated background)
- choice of crystals

Neutron optics: choppers (primary spect.)

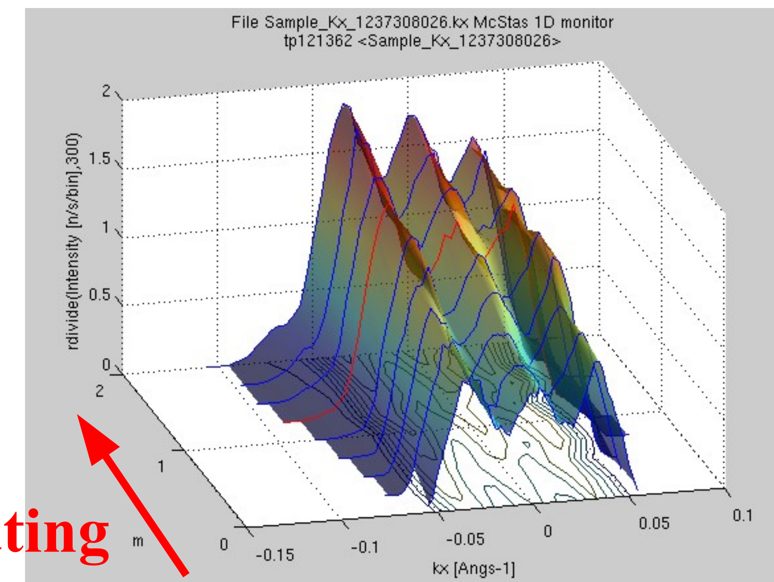




200 Al blades
Gd absorber
Replaced with NiTi

Rotation 10000 rpm

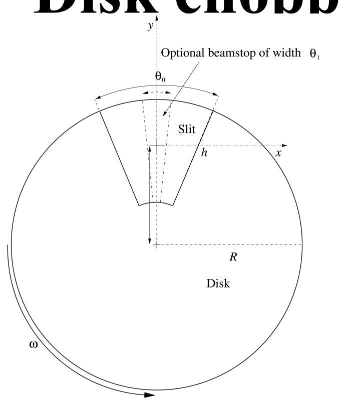
Here, we change the **Fermi chopper** coating to increase the flux at the sample position.

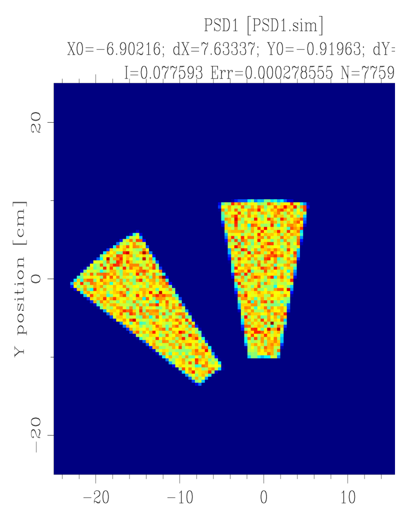


Coating

Angle

Disk choppers

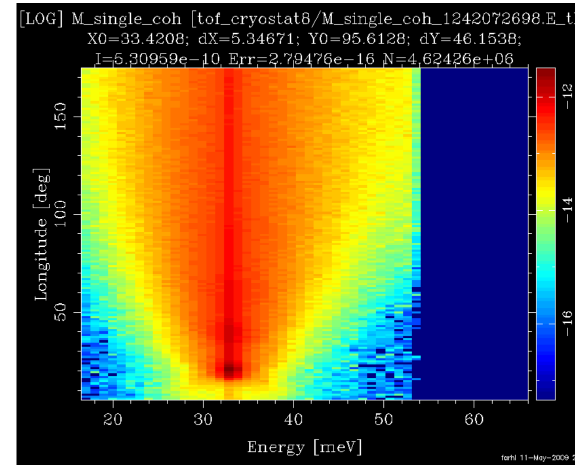




Sample environments: hot/cold, magnets

Sample is usually studied at low or high temperatures. **Cryostats** and **furnaces**
Must not generate too much background (all materials in the beam scatter, not only sample)..

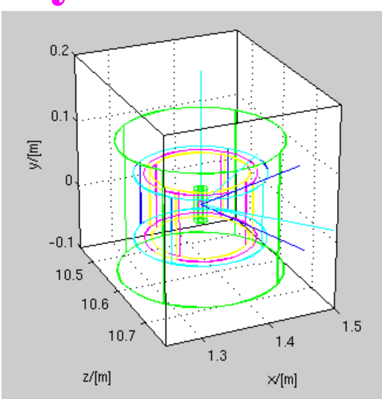
Coherent single scattering

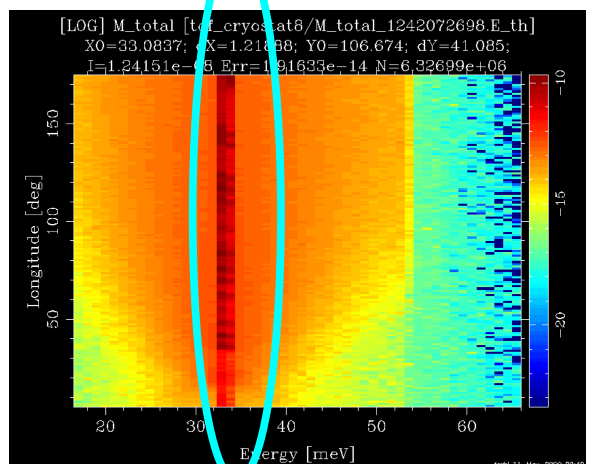


Liquid Rb $S_{coh}(Q,\omega)$

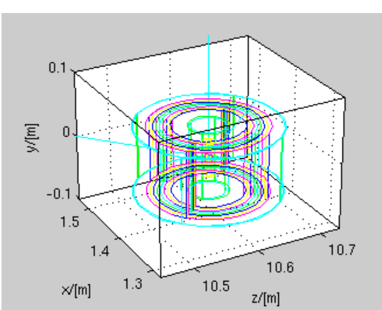
TOF E0=33 meV. Liquid Rb.

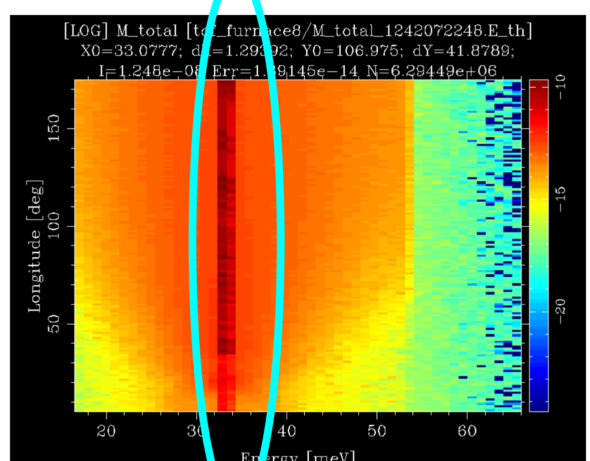
Cryostat: 4 Al shields





Furnace: 12 shields (Al, Nb)





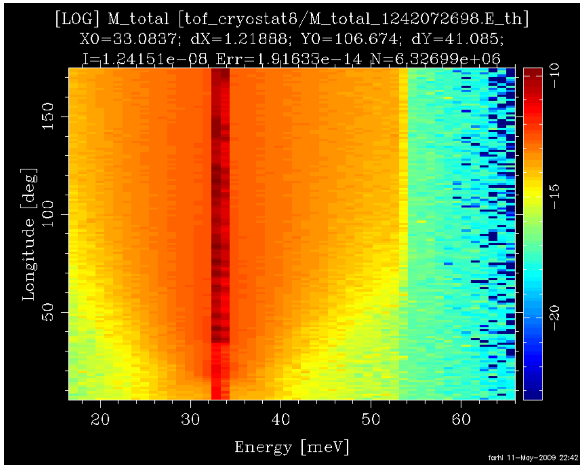
Question for you:
How to remove this contribution ?

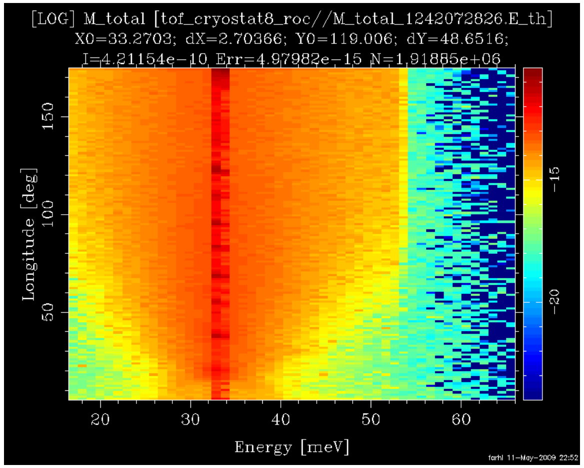
Let's simulate this...

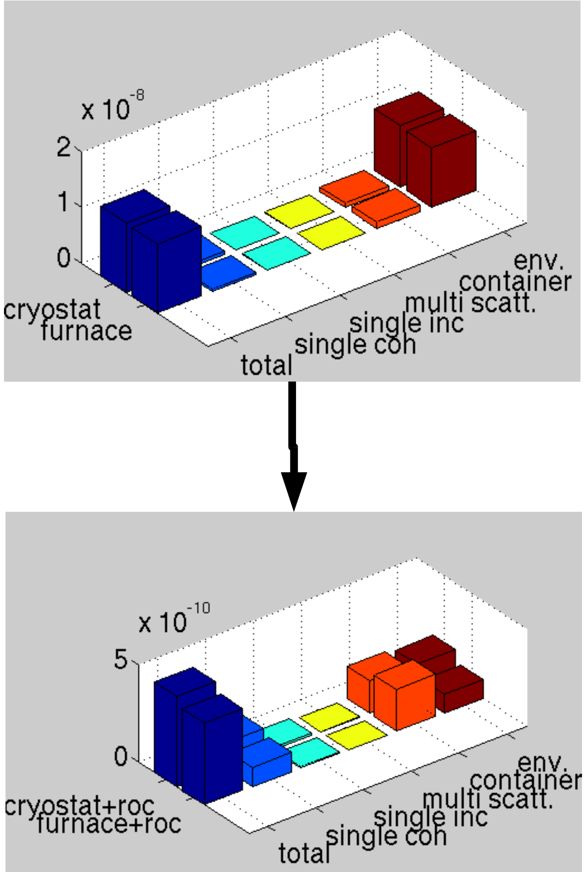
Simulated total signal
Log scales

Sample environments: removing some background

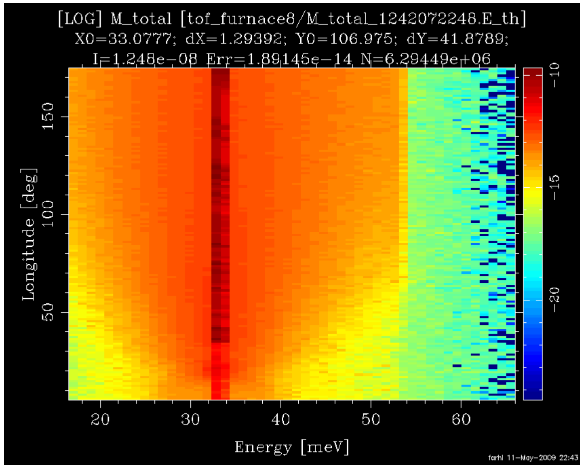
Cryostat: 4 Al shields

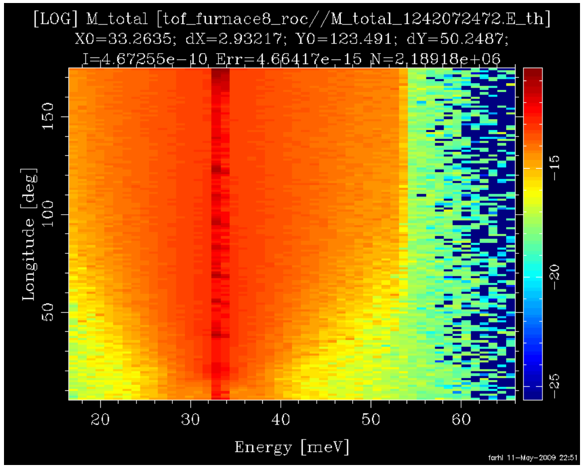






Furnace: 12 shields (Al, Nb)





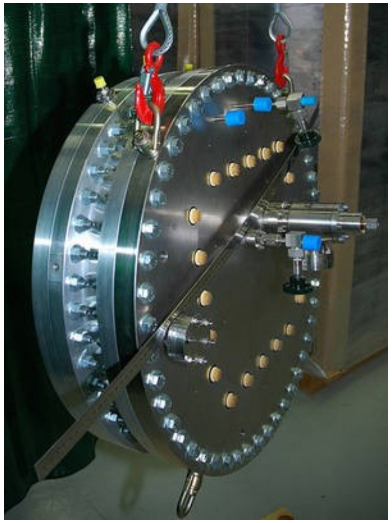
With ROC, mainly remains container. Physics becomes visible.

Neutron detectors

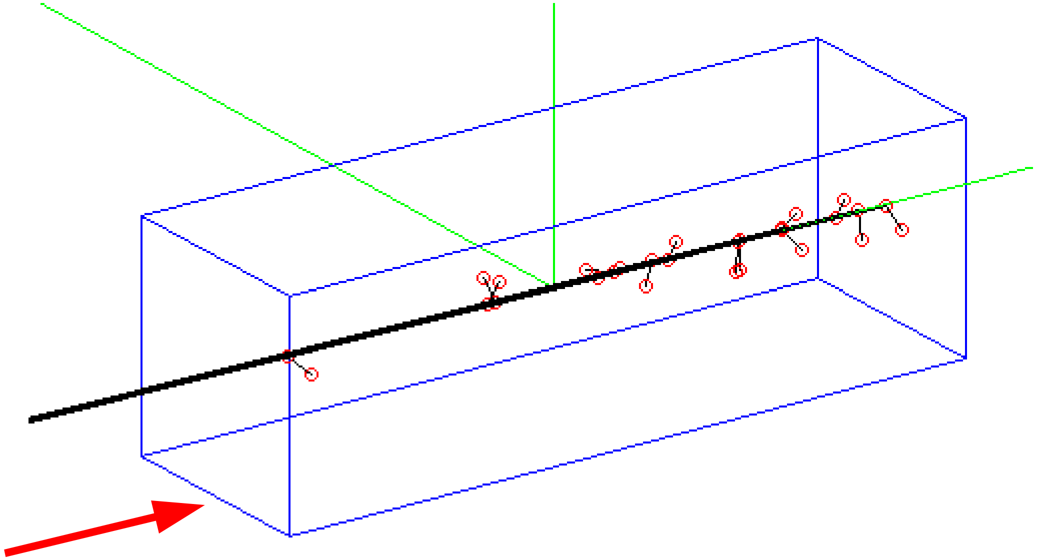
Detector model for MWPC: visualize (p,t) charge drift.

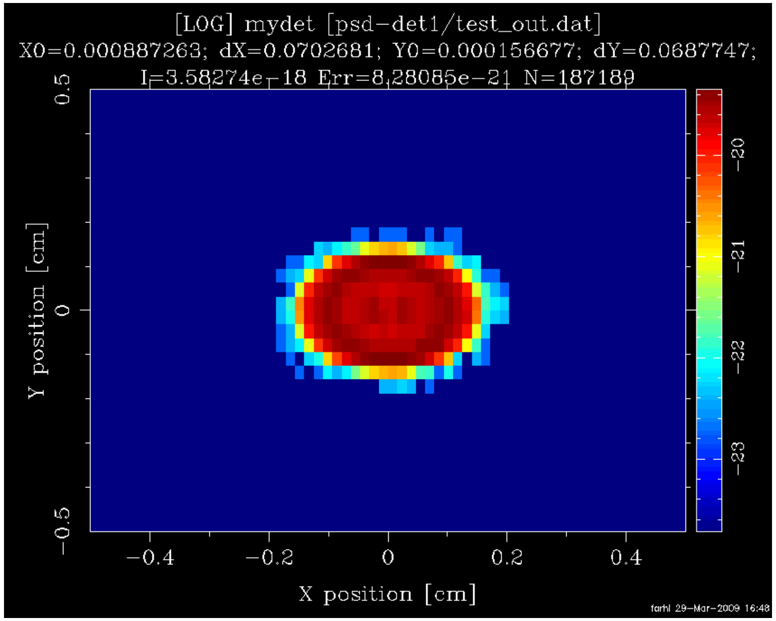
Can study:

- detector spatial resolution
- estimate detector saturation
- background generated from detector housing.



Detection area 1x1 cm, He 5 bars, CF4 1 bar.





Resolution 0.4 cm

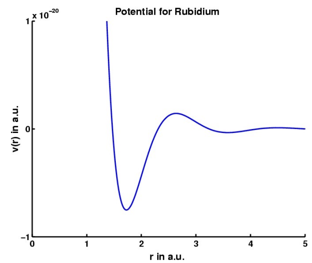
Virtual experiment: definition

Virtual experiment = simulation of sample + simulation of instrument

Molecular Dynamics

Inter-atomic potential u(r)

$$\vec{F} = -\nabla u(\vec{r}) = m\vec{\gamma}$$



Ab-initio (VASP)

Pseudo-potential

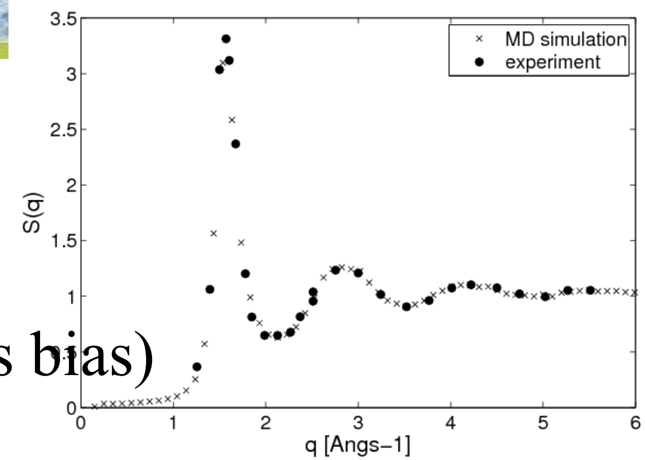
Experiments (corrected)

R, v → *nMoldyn* → **S(Q,ω)**

This step is done prior to the virtual experiment.
Computationally intensive (e.g. Use clusters).

McStas provides a few sample S(Q,w).
Materials I'm working on: **Rb**, Au, Al, Bi, Hg, **In**, Pb, Se, Si, Ti, Tl

Virtual experiment: *l*-Rb



Experiments: Copley (PRA 1974) TOF and TAS

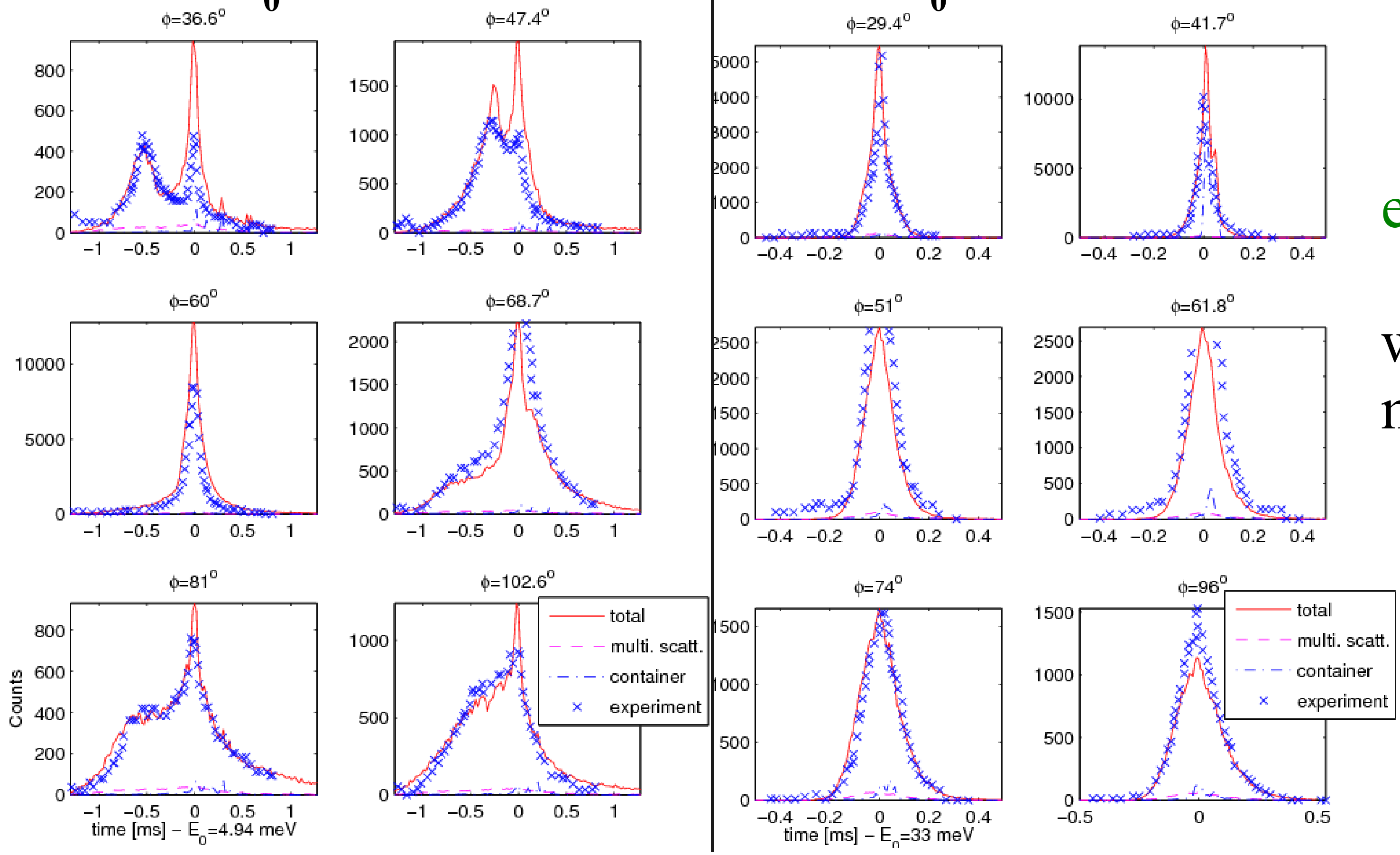
Simulation: 520 atoms in classical MD for 50 ps

T=315 K, c=1300 m/s, D=0.23 Å^2/ps

Comparison with raw results (to avoid data analysis bias)

Structure: **OK**

E_0=4 meV E_0=33 meV



Dynamics *vs* raw experimental results: **OK** with container and multiple scattering.

Parameters:

HybridTOF geometry

CP5 reactor power

Kahl 2-body potential

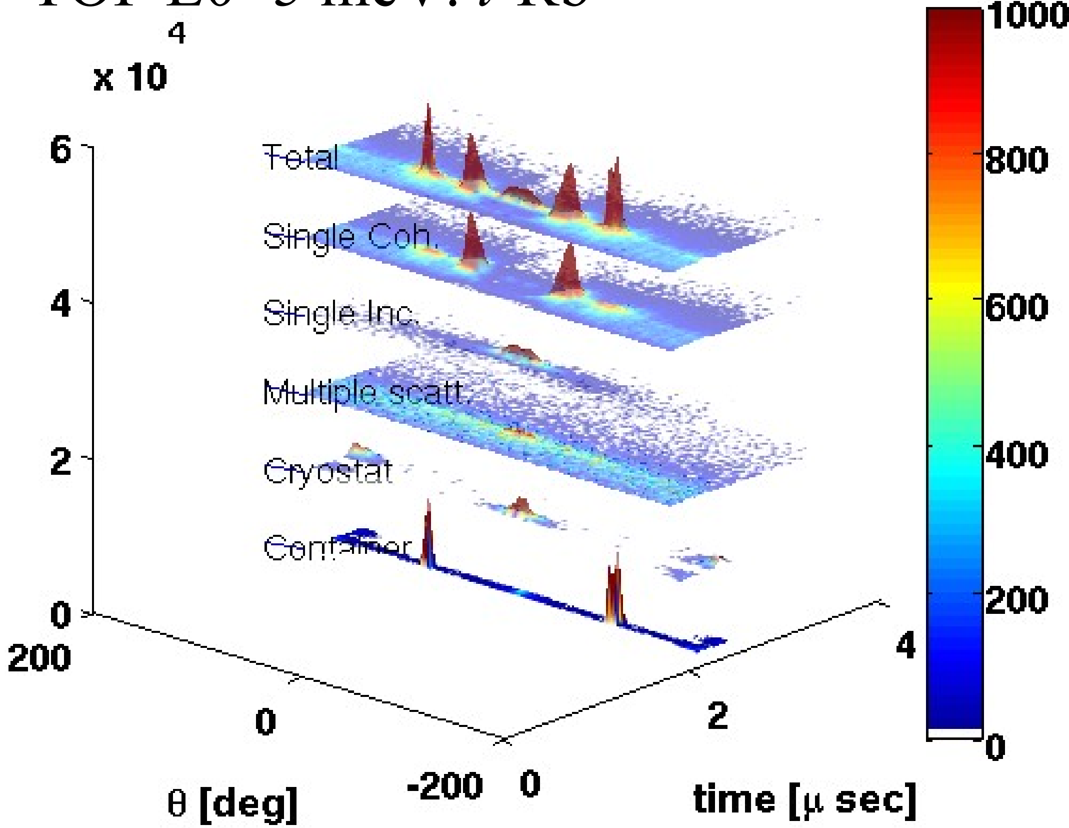
r=1.3 Å value for Rb

Example: liquid rubidium

COMPONENT Sample=**Isotropic_Sqw**(
radius_o = 0.01, yheight = 0.055,
Sqw_coh=*”Rb_liq_coh.sqw”*, Sqw_inc=*”Rb_liq_inc.sqw”)*
AT (0, 0, 0) RELATIVE Sample_pos

```
TRACE

COMPONENT Source
COMPONENT Sample=Isotropic_Sqw()
  AT 1.5 m RELATIVE Source
COMPONENT Collimator_radial
COMPONENT MonitorTotal WHEN SCATTERED
COMPONENT MonitorCoh WHEN coherent
COMPONENT MonitorInc WHEN incoherent
COMPONENT MonitorMulti WHEN SCATTERED>1

END
```

TOF E0=5 meV. *l*-Rb



McStas code (schematic)

We can separate contributions from each part of the simulation (not possible in real life)

Example: liquid indium

Indium: σ_{abs}=193 b ; σ_{scatt}=2.6 b

very few previous studies

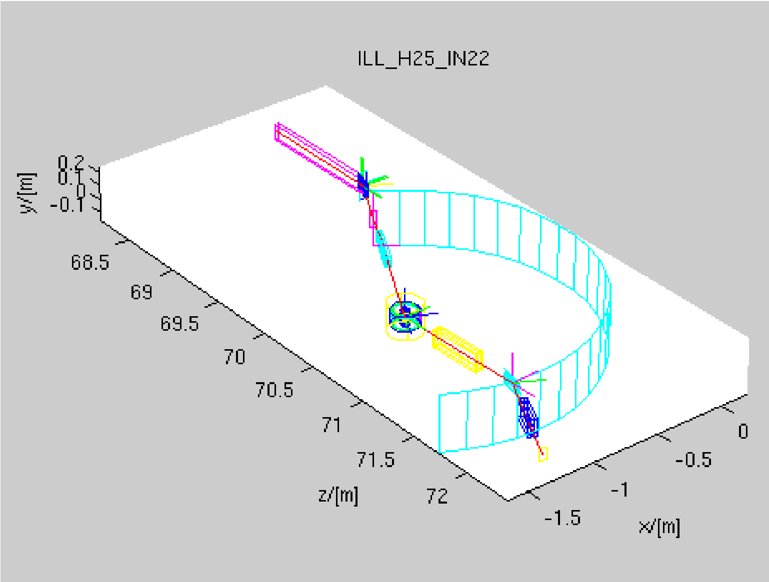
Experiment performed on IN22@ILL TAS

a 'virtual *vs* real experiment'

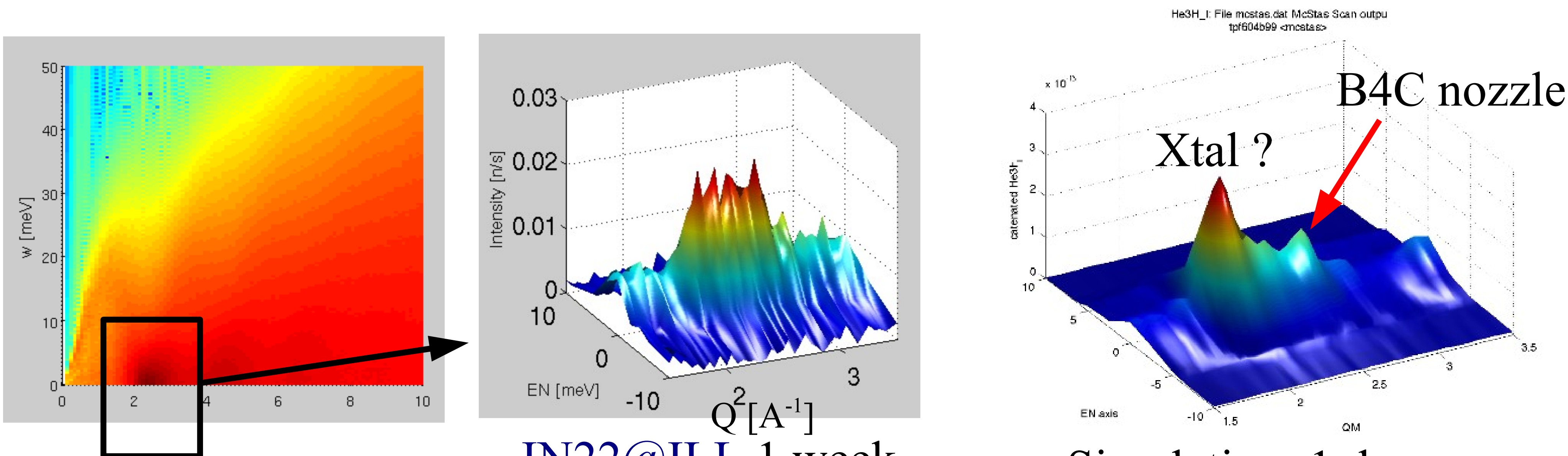
Simulation: *ab-initio* using VASP, 200 atoms for 36 ps

levitation
furnace+laser
ϕ=2 mm
no container

simulation with
absolute flux



Example: liquid indium

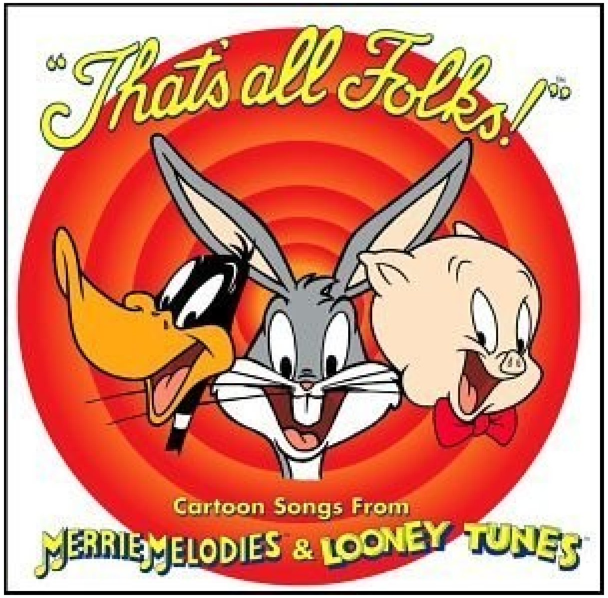


IN22@ILL 1 week

Simulation: 1 day

Not yet perfect: simulations of B4C nozzle must be improved.
Virtual sample may be slightly crystallized.
Main features and absolute intensity reproduced.

Without simulation, the experiment would have been a failure.


"That's all Folks!"
Cartoon Songs From
MERRIE MELODIES & LOONEY TUNES