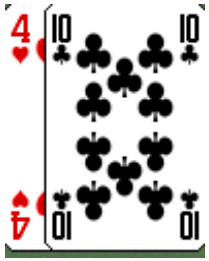
Virtual experiments:
how far can we go ?

Emmanuel Farhi (ILL/DS/CS)
Virginie Hugouvieux (ILL/INRA)
Mark Johnson (ILL)

What are Monte Carlo methods ?

- Use random generators (play poker/roulette)
  (Ulam, von Neumann)
- Explore a complex and large phase space



- Integrates microscopic random events into measurable quantities
  not a usual regular sampling integration

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

- *Metropolis* algorithm: model energy gap E as a probability

$$p \propto e^{-E/kT}$$

- Integrals converge faster than *any* other method (for $d > 3$)
  when using *enough* independent events (central limit theorem)

F. James, *Rep. Prog. Phys.*, Vol. **43** (1980) 1145.

Grids and Clusters

Gridding

McStas may run on heterogeneous grids
for scans and repeated simulations

Clusters

McStas has native **MPI** implementation (MPICH preferred)
Has 100 % efficiency

Collecting/Merging data sets

The '**mcformat**' command merges and converts data files

What are MC codes used for today ?

Most MC codes in neutronics are used for:

- Sources computations
- Guides studies
- Instrument inter comparisons using 'idealized' samples
- Basic instrument characterization (flux, resolution)

Users now look for even better accuracy in the models.
Background estimate required.

Missing bits ?

Sources:	**OK**
Optics:	**OK** (satisfactory)
Monitors:	**OK but not realistic**
Samples:	**Not OK**

Present MC packages lack accurate sample models

- Excitations in Liquids and Crystals
- Accurate Structures

They usually have:

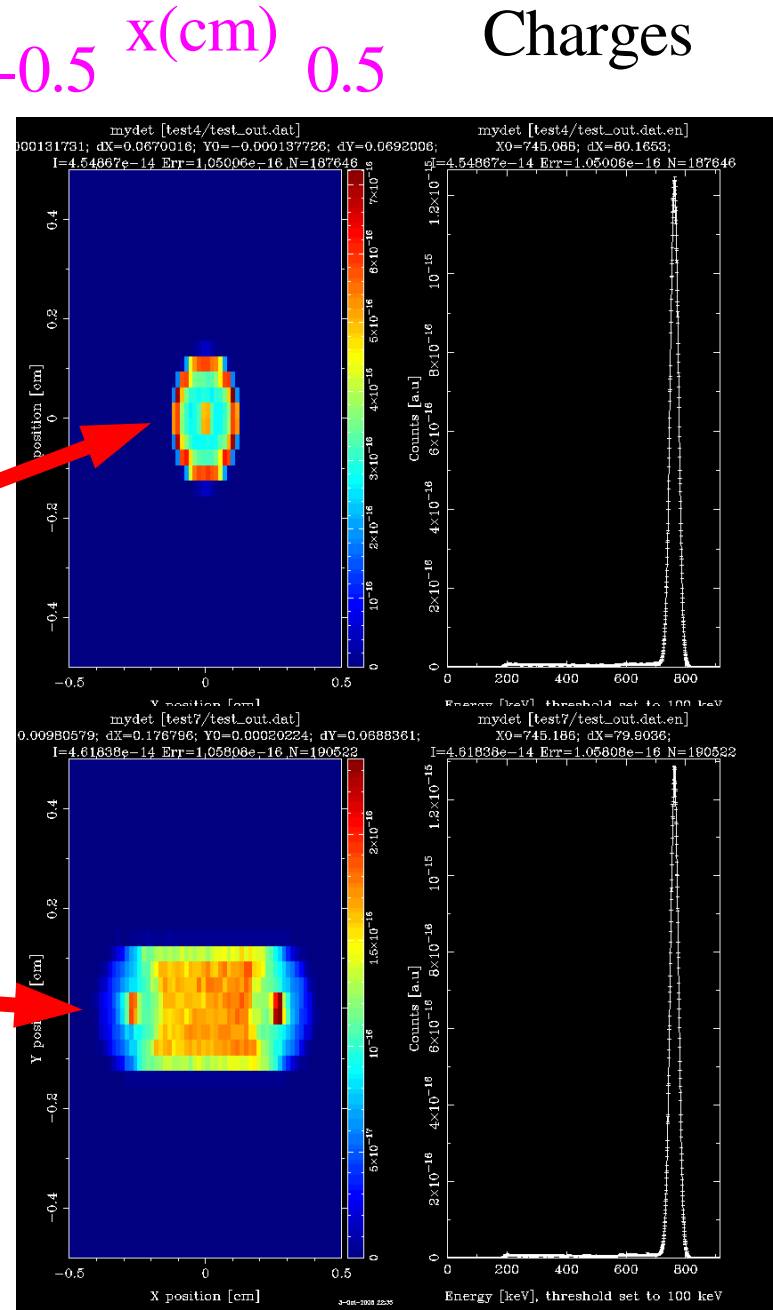
- Vanadium-like stuff
- Simple powders
- Basic/specific components (phonon-like, ...)

Virtual experiments are still hardly comparable with experiments

An accurate detector model

New McStas detector component: PSD_Detector

Flat and banana shaped PSD
Include thickness
Handle all kind of gas mix
Handle charges drift in the gas
-> parallax effects
Many other features... (boarders

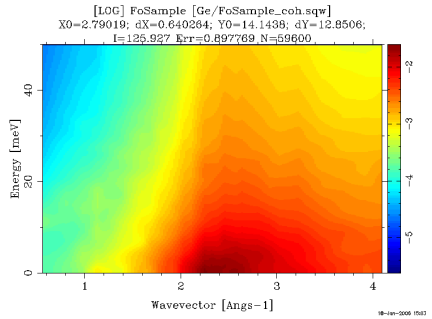


Contributed by T. van Vuure
Collaboration with ILL detector group

Isotropic material (liquid) component for *McStas*

`Isotropic_Sqw` sample component for *McStas*

- coherent/incoherent scattering,
- elastic and inelastic scattering,
- absorption (with secondary extinction)
- multiple scattering
- requires an *Sqw* table as input for **inelastic** scattering
- may use *Fullprof, Crystallographica, etc* files for **powders**
- geometry is a box, cylinder, sphere – filled or hollow
- can be arranged in concentric geometry (sample env.)



l-Ge coh (log)

A bit of theory

See Egelstaff or H. Fischer, *Rev. Prog. Phys.* **69** (2006) 233

Neutronist's Mantra

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma}{4\pi}\frac{k_f}{k_i}NS(q,\omega)$$

Holy Book (Squires)

Effective cross section for scattered intensity

$$\hat{\sigma} = \iint \frac{d^2\sigma}{d\Omega dE_f} d\Omega dE_f$$

V.F. Sears. Adv. Phys., 24, 1, 1975.

We like to play games in (q,ω) space

$$\frac{d\Omega}{d\theta} = -2\pi sin\theta$$

$$\frac{dq}{d\theta} = -\frac{k_i k_f sin\theta}{q}$$

Effective cross section in (q,ω) space

$$\hat{\sigma} = \sigma \iint \frac{S(q,\omega)q}{2k_i^2} dq d\omega$$

Probability to interact

$$p = \mathrm{e}^{-\rho\hat{\sigma}x}$$

Scattering distribution

$$S(q,\omega)$$

A bit of theory (2)

This method requires to normalize S(q,ω)

structure factor

$$g(r) - 1 = \frac{1}{2\pi^2 \rho} \int_0^\infty q^2 [S(q) - 1] \frac{sin(qr)}{qr} dq$$

$g(r \to 0) = 0$

$$\int_0^\infty q^2 [S(q) - 1] dq = -2\pi^2 \rho$$

gives |S| = f(ρ)

Probability functions sampled from S(q,ω)

$g_\omega(\omega)$ $g_q(q|\omega)$

Implementation similar to MSC/MSCAT and DISCUS:

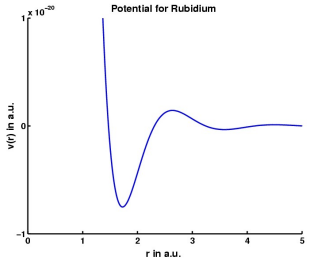
- easy to obtain (open source/GPL)
- easy to use (doc, part of McStas)

Prepare sample model from S(|Q|,ω)

Molecular Dynamics

Inter-atomic potential u(r)

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



Ab-initio (VASP)

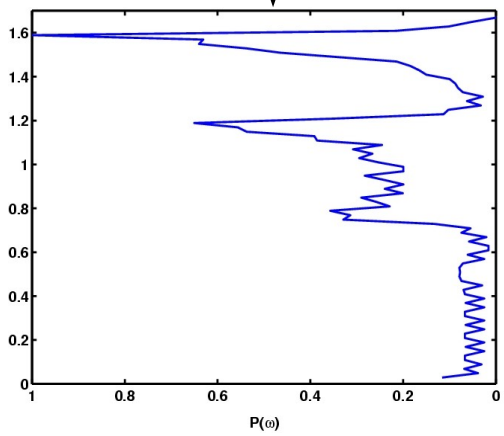
Pseudo-potential

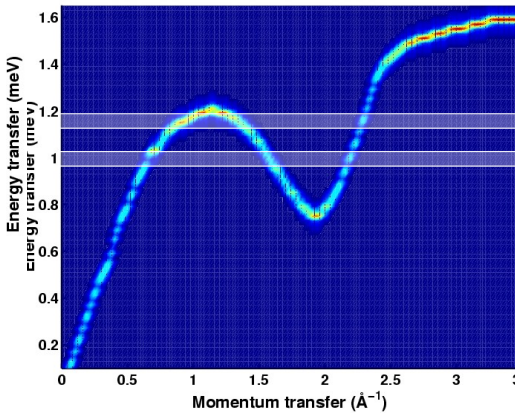
Experiments (corrected)

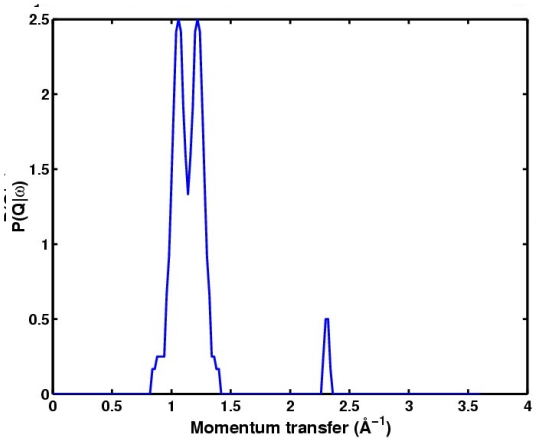
R, v → *nMoldyn* → S(Q,ω)

S(Q,ω) sampling

For each ω, compute DOS-like $g_\omega = \sum_Q S(Q,\omega)$







For each $\omega = \omega_i$, compute g_q

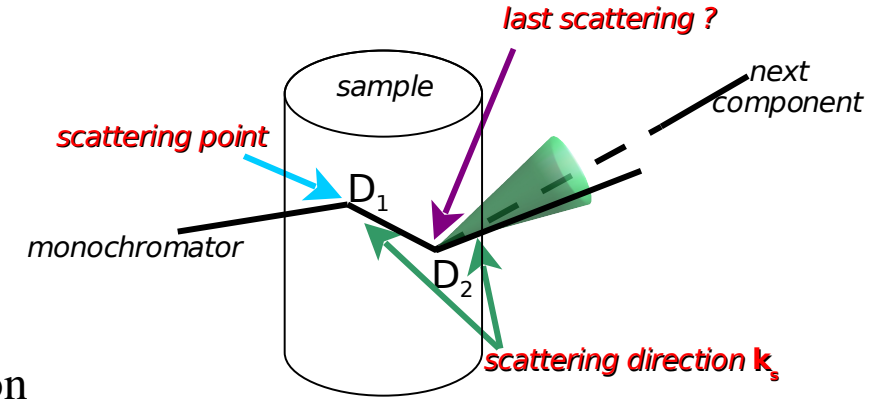
From V. Hugouvieux, *PhD (2004)*

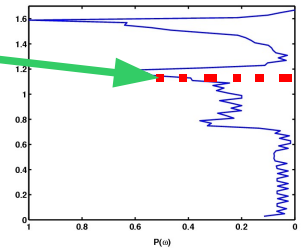
Propagation in sample

Scattering events loop :

- compute the effective cross section $\hat{\sigma}$ for the neutron k_i
- choose the scattering point D_i along trajectory :

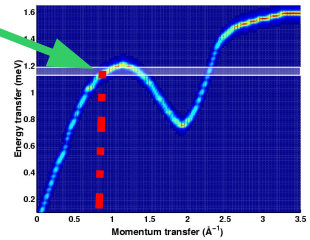
  $1-e^{-\mu x}$ with $\mu=\rho\sigma$ and 2nd extinction
- choose if coherent or incoherent scatt. and weight absorption
- choose ω randomly in the DOS g_ω
- choose either ω or -ω (detailed balance)
- choose q randomly in a probability table $g_q(q \mid)$
- check selection rules and get $|k_f|$: $\hbar\omega = k_i^2 - k_f^2$
- solve scattering direction : $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f}$
- compute the distance *d* to sample exit
- scatter again until the neutron exits the sample





ω

$g_\omega(\omega)$



ω

$g_q(q|\omega)$

Q

$S(Q,\omega)$

Hugouvieux *et al. Physica B*, **350** (2004) 151 and NIM A (submitted, 2006)

Obtaining S(q,ω)

Current S(q,ω) files from the McStas distribution:

- Rb (Copley) and Classical MD (Hugouvieux)
- Ge *ab-initio* MD (Hugouvieux)
- Cs (Dorner) and ab-initio MD (Farhi, on going)
- Ne (Sears, no phonons)
- He (model)
- All ICSD powders

Liquid
Gas
Powder
Glass
Polymers

On going studies:

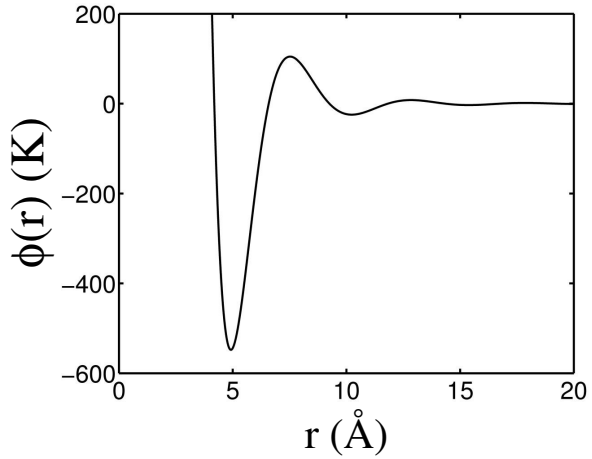
- Propanol Classical MD (Gonzales)
- Water (temptatives)
- Au, Al, Bi, Hg, In, Pb, Se, Si, Ti, Tl ab-initio MD (Farhi)

Virtual experiment : the sample model for l-*Rb*

Liquid rubidium, 350 K

- Agrees with experiments from Copley, *Phys. Rev.* A, **9** (1974) 1656.
- 2-body potential by Kahl, *Phys. Rev.* A **46** (1992) 3255.
- S(q,ω) computed by V. Hugouvieux, PhD (2004)
- classical MD with 520 atoms.

Interatomic potential



$\sigma_{abs} = 0.38$ b

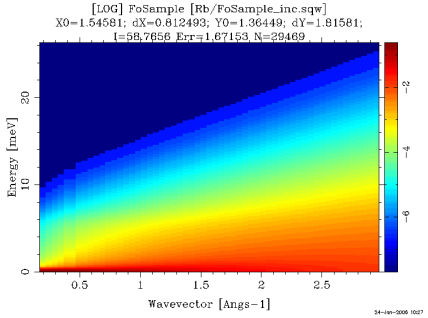
$\sigma_{coh} = 6.32$ b

$\sigma_{inc} = 0.5$ b

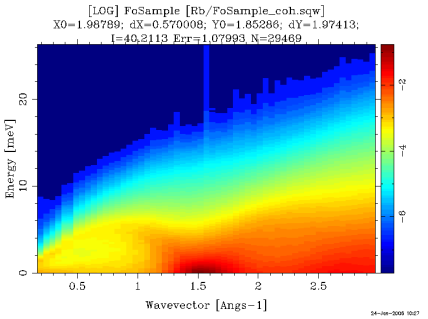
$T_m = 312$ K

$T_b = 961$ K

l-Rb inc (log)



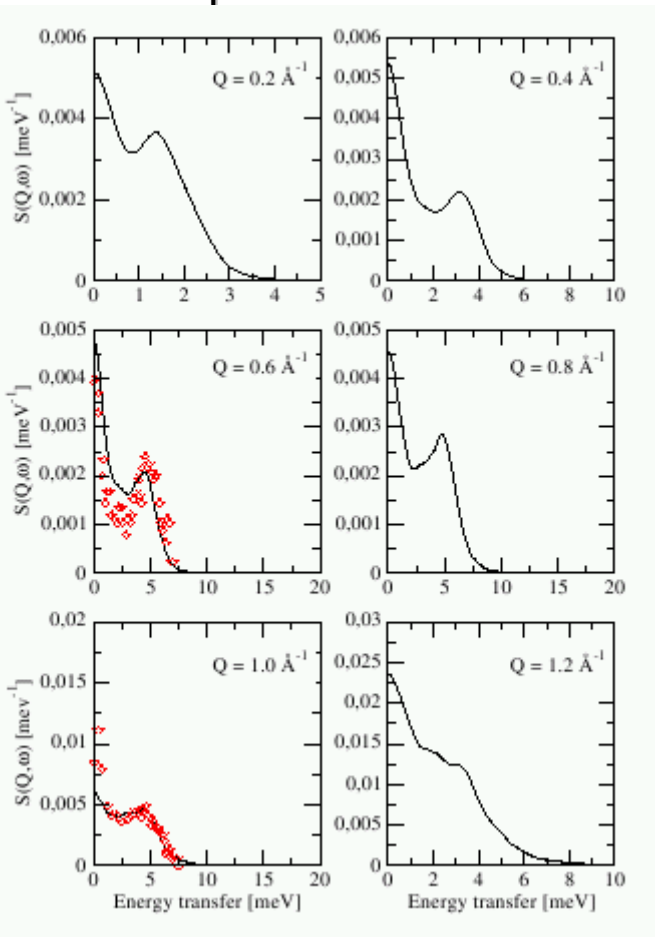
l-Rb coh (log)



From ***V. Hugouvieux***

Dynamic structure factor :
Q < 1Å

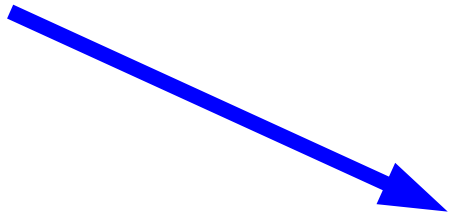
phonon



Farhi – ILL/DS/CS

Inserting the sample

```
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
```



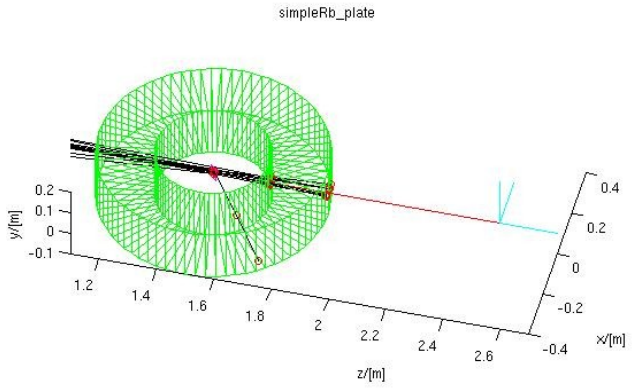
```
TRACE

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
```

Single sample : the instrument and monitors

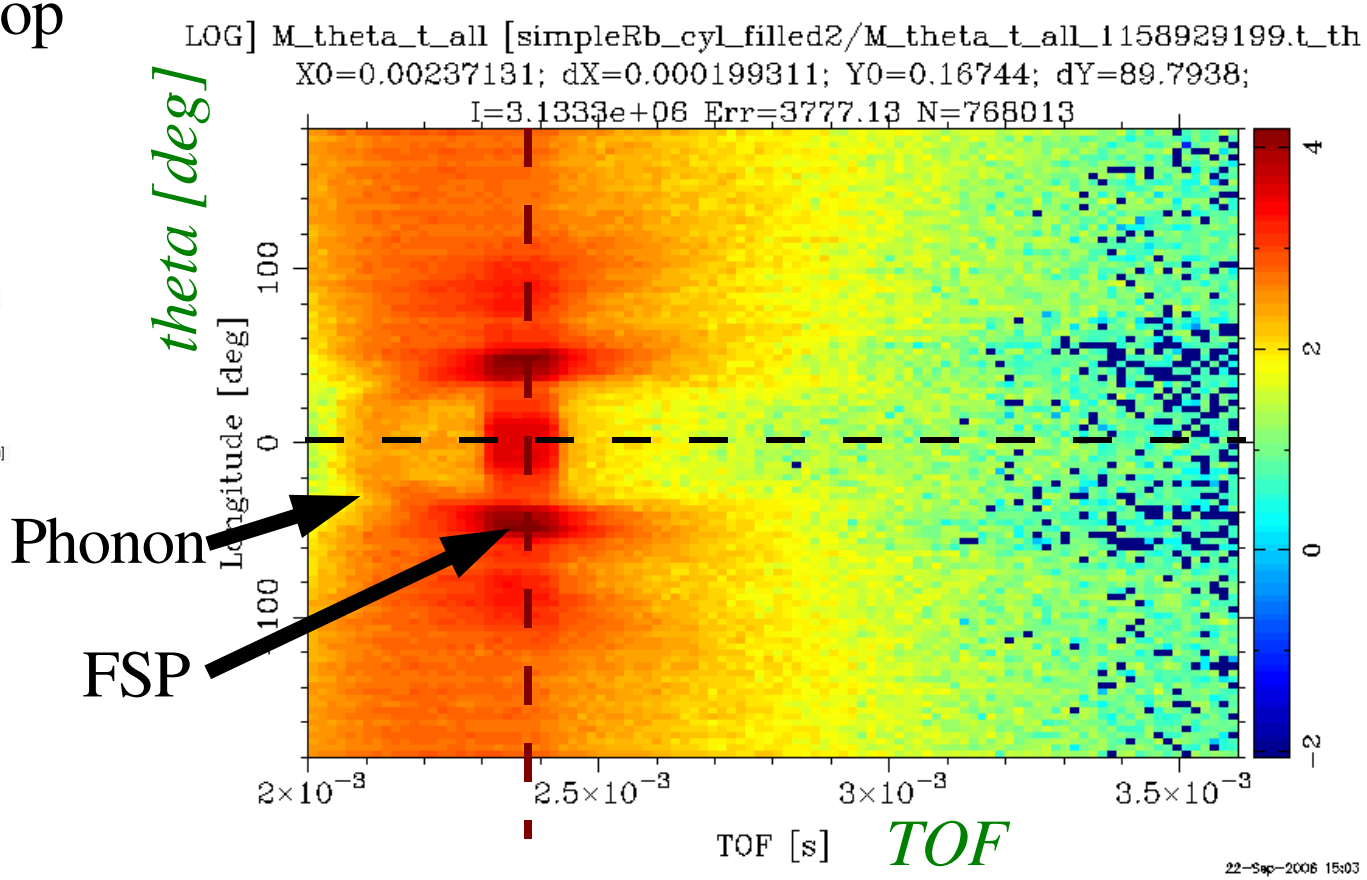
We start with a virtual experiment containing just:

l-Rb

- a source: beam 2 x 2 cm (PSI cold spectra)
- a sample *l*-Rb (cylinder ϕ=2 cm at 1.5 m)
- surrounding radial collimator (IN5 model)
- monitors and beam stop



λ=3.95 A^{-1}

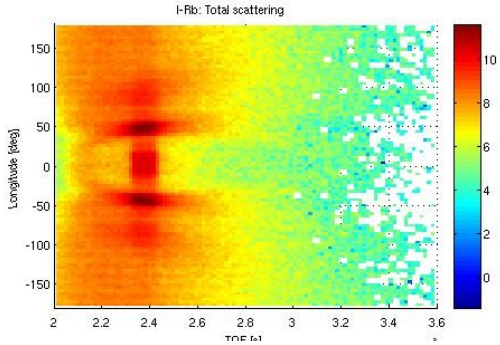


Computation time: about 10^4 events/s at final detector.

Single sample : coherent/incoherent signal

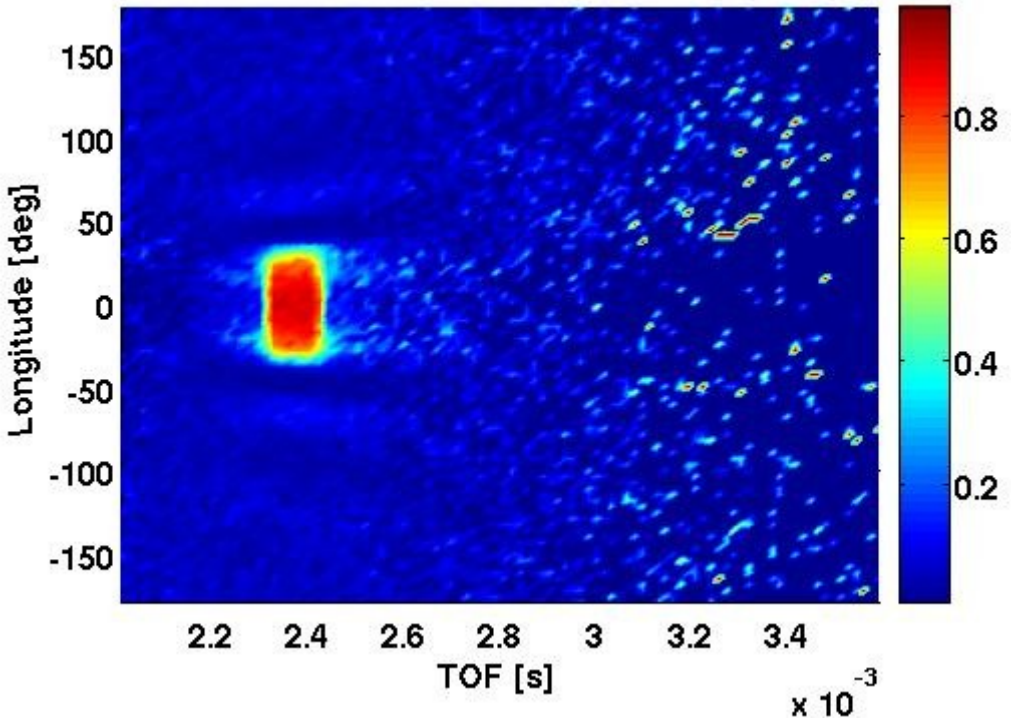
Total signal (log scale)

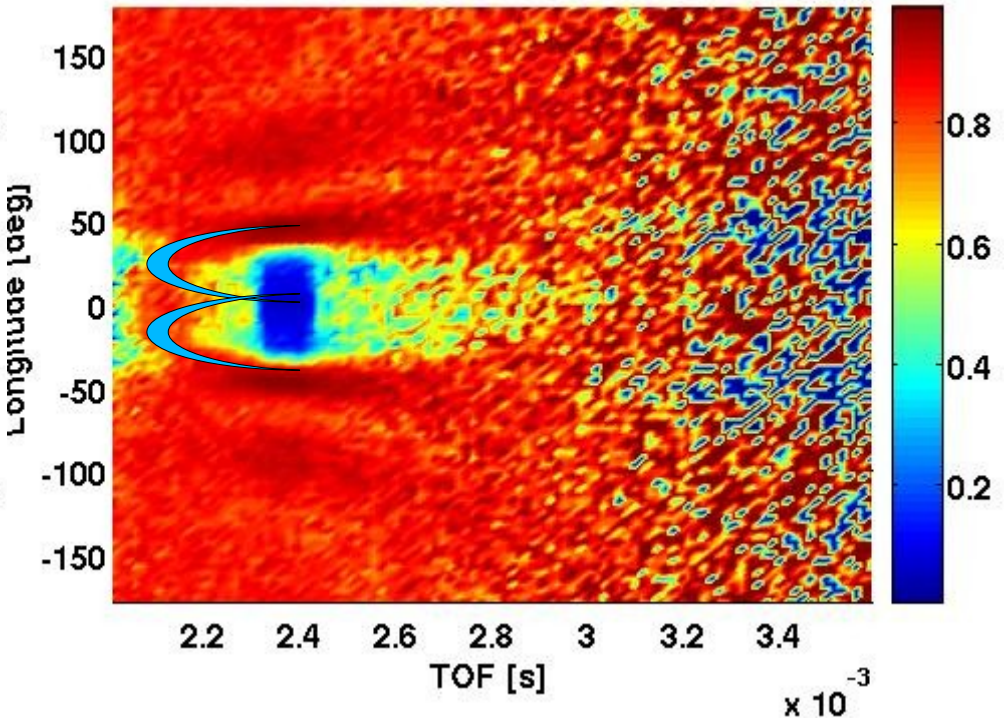
l-Rb



Ratio:
single inc/all

Ratio:
single coh/all





inc: About 10 % except at low q, ω

coh: About 85-95 %

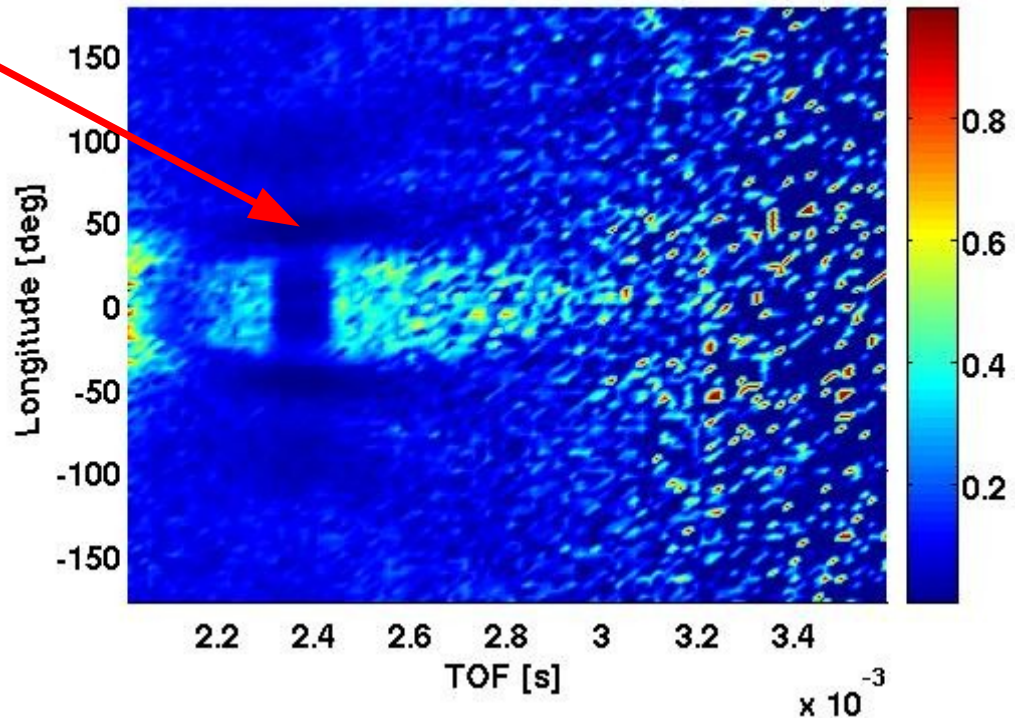
Single sample : multiple scattering

l-Rb

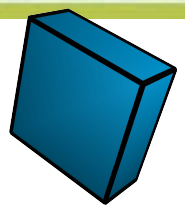
Extract multiple scattering events:

- About 5-10 %.
- Locally up to 40 % at low *q*.
- Lower than 3 % on *max(S(q))*

Ratio:
multi/all



Single sample : sample geometry

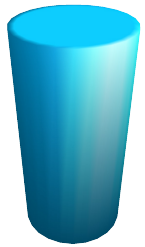


l-Rb: plate 1cm thick

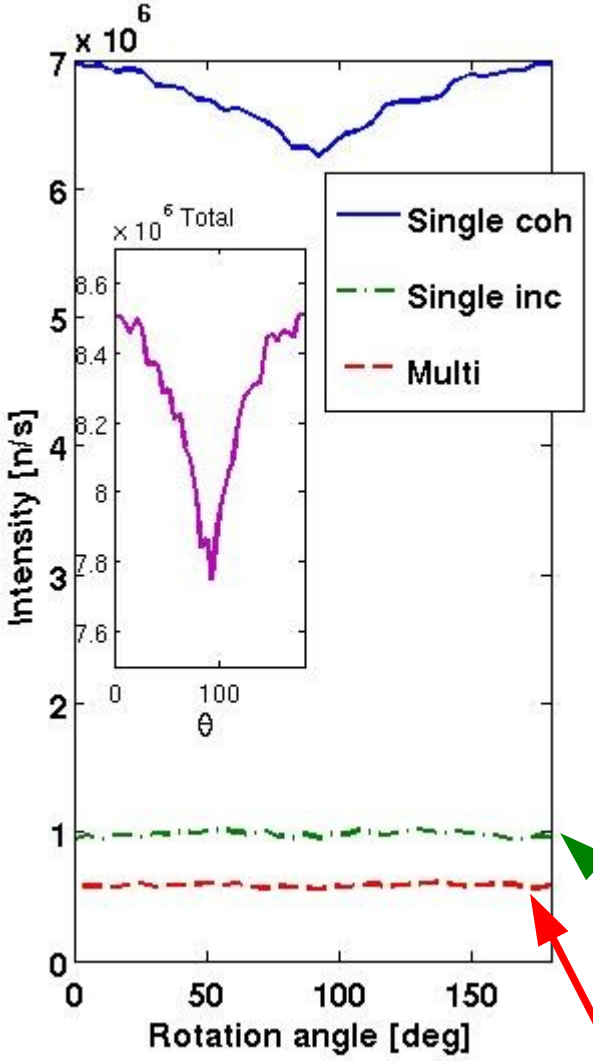
Determine best sample geometry ?

Plate orientation

Sample dimension



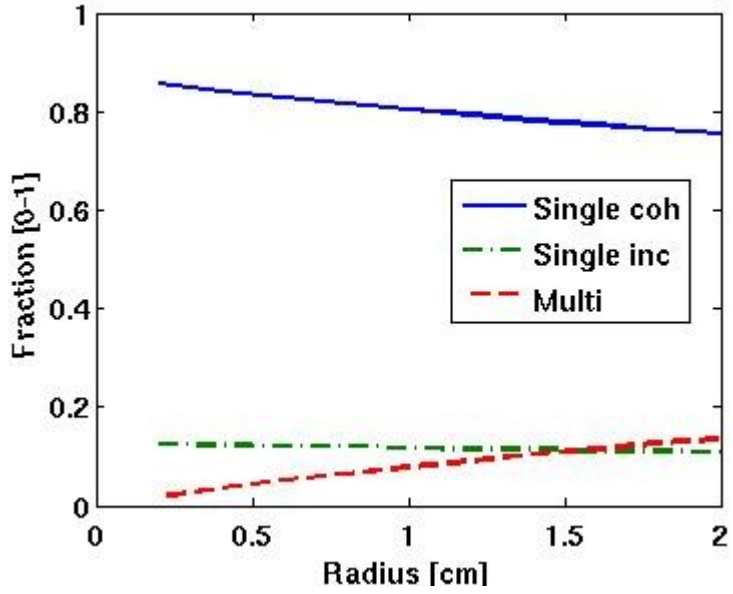
l-Rb: filled cylinder



-10 %

14.6 %

8.7 %



Conclusion:

Multiple scattering is usually over-estimated

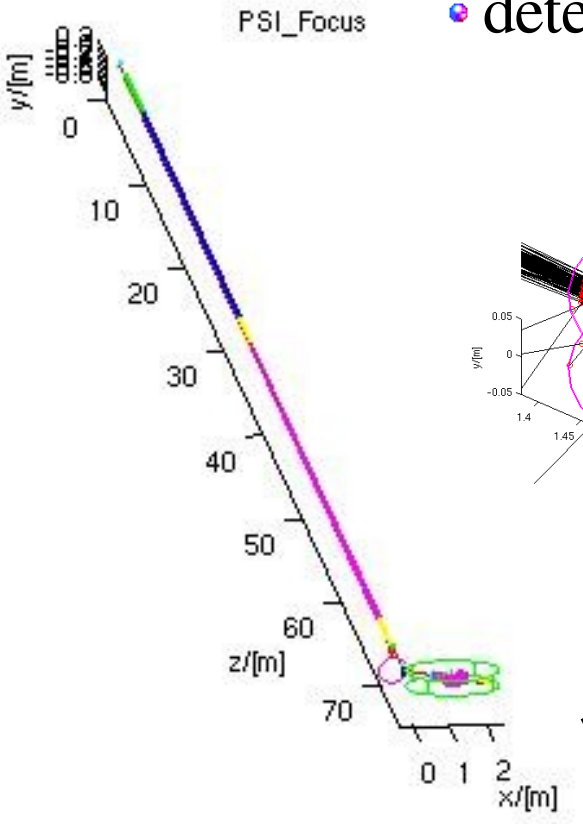
Better get bigger sample !

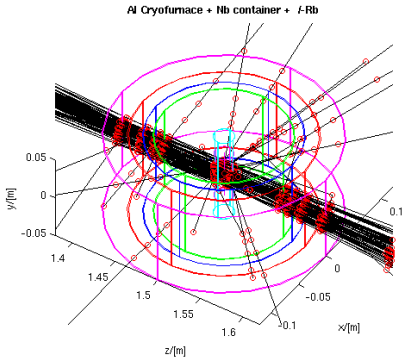
Focus@PSI : the model

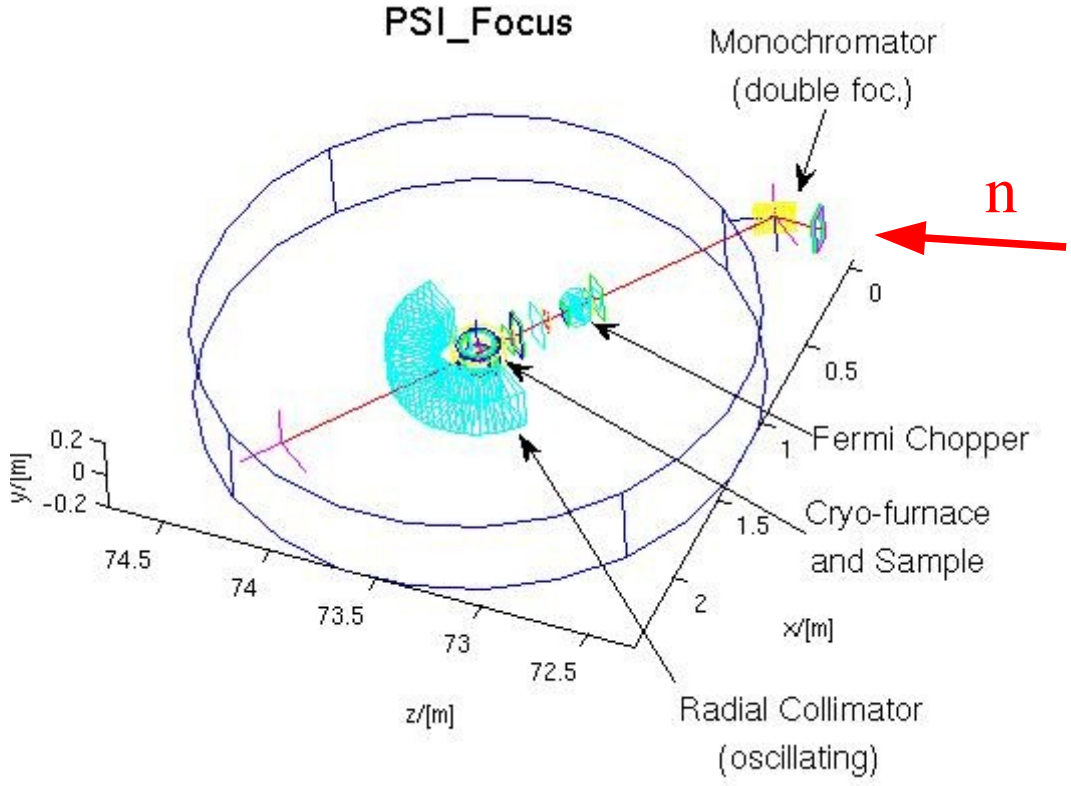
The instrument model is now the ToF instrument Focus at PSI

- Source: converging beam at Fermi Chopper, PSI cold spectra
- Guide and background chopper
- curved monochromator
- Fermi chopper
- furnace
- sample *l*-Rb
- detectors

Uwe Filges





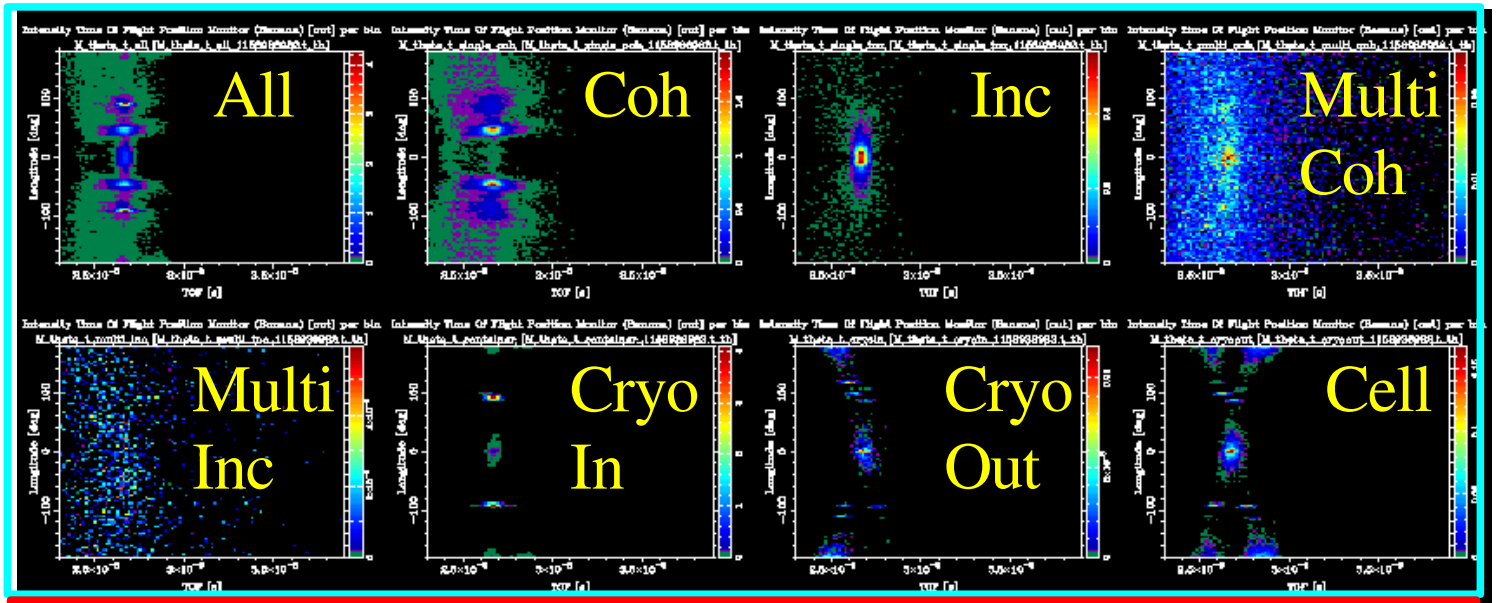


Computation time: 100 events/s at final detector

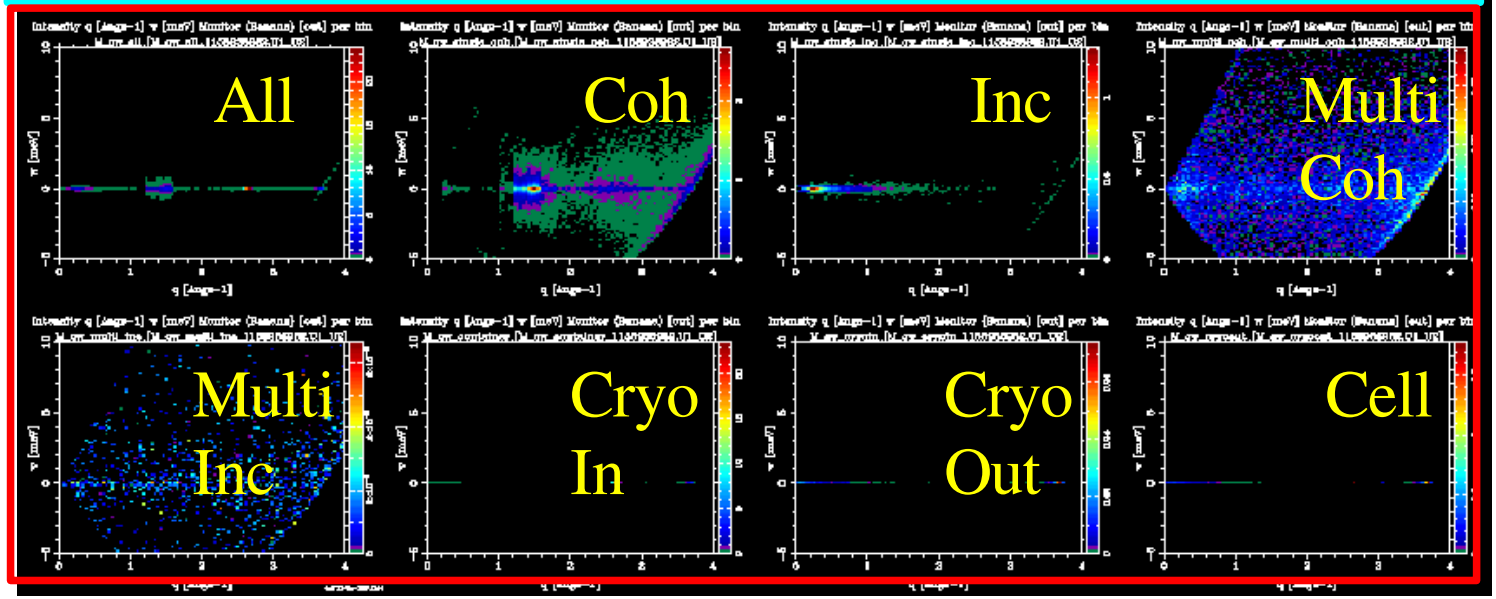
Typical 1 h

Virtual Experiment raw results

θ ToF



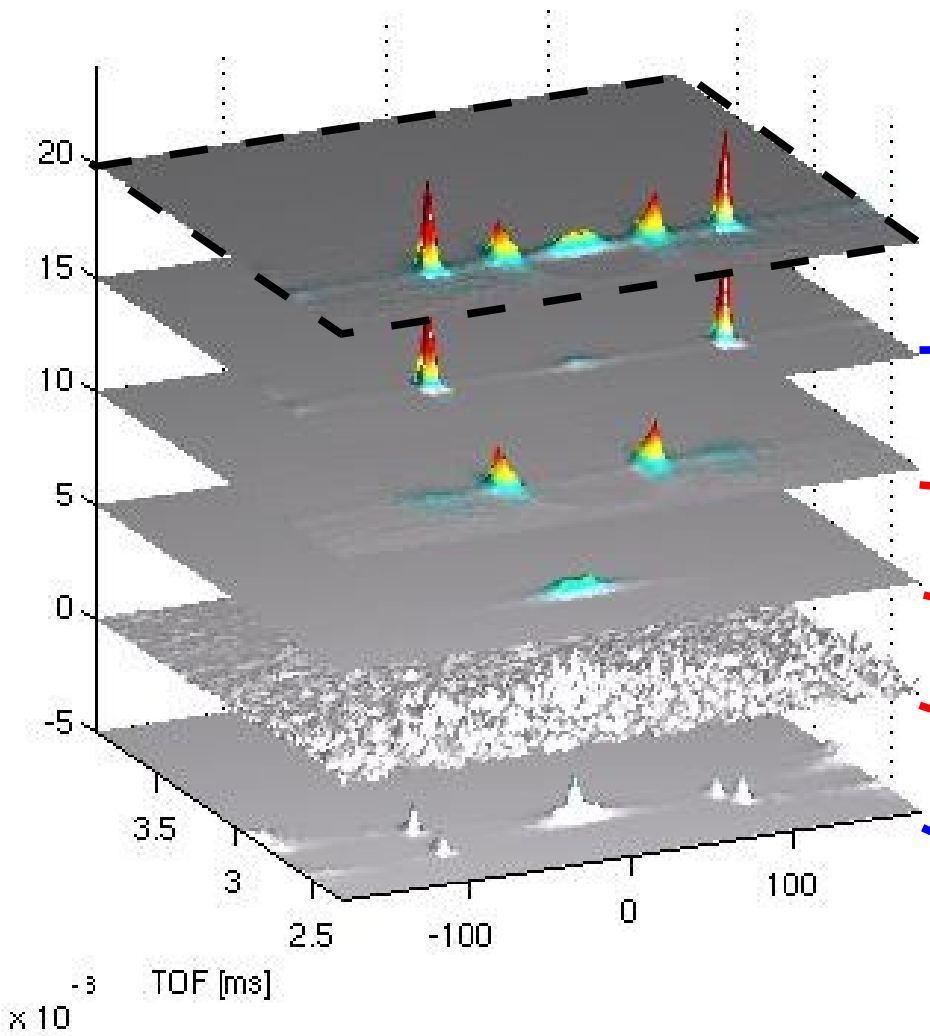
q ω



Focus@PSI
l-Rb
λ=3.4 Å
beam:
3.8 x 7 cm

Sample Environment : labelling contributions

Focus@PSI
l-Rb
λ=3.4 Å
beam:
3.8 x 7 cm



Total signal

Container (Nb)

Coherent (l-Rb)

Incoherent (l-Rb)

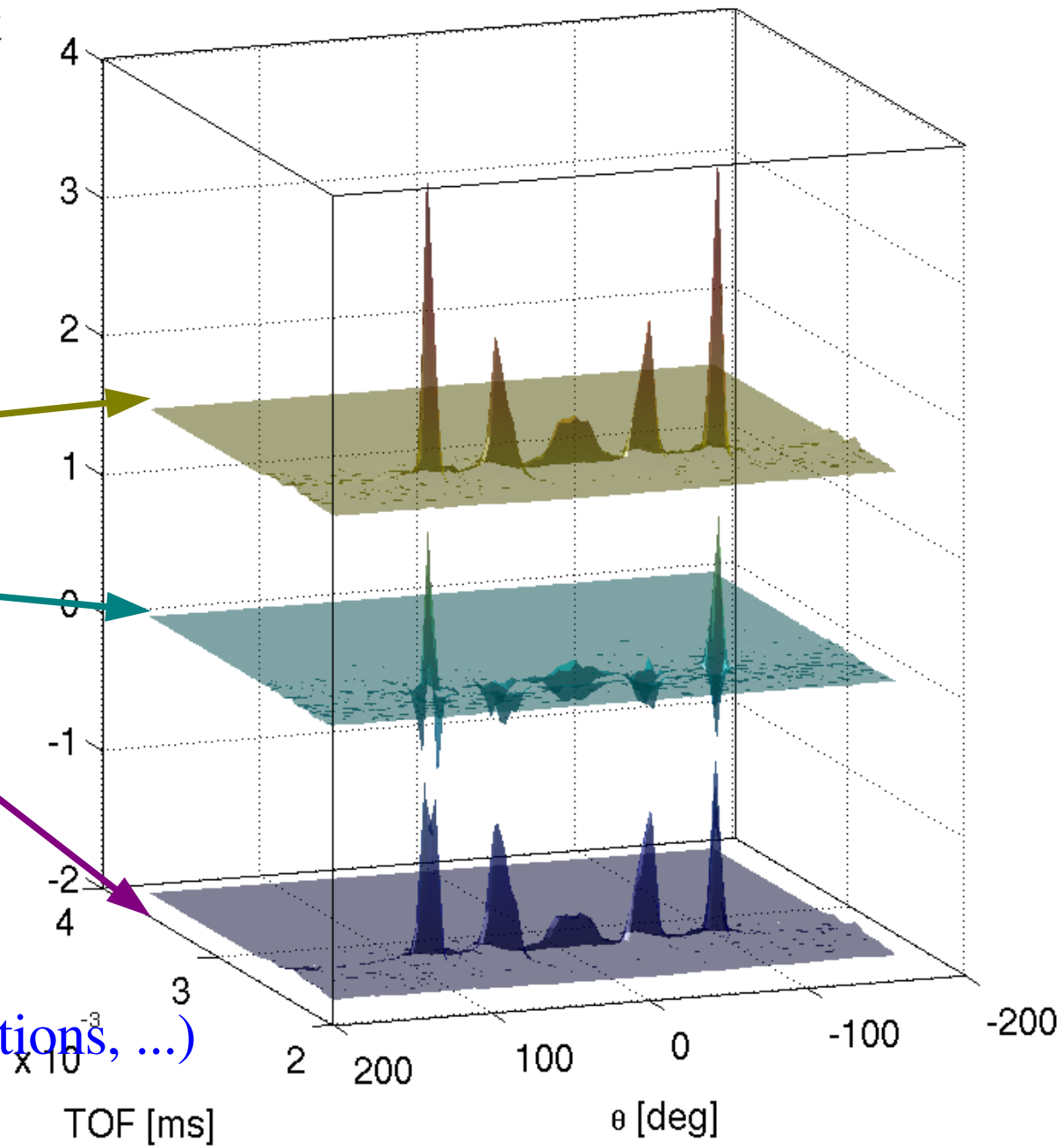
Multi. Scatt. *100

Cryo-furnace (Al) *10

Focus@PSI : Effect of instrument (example)

Difference between:

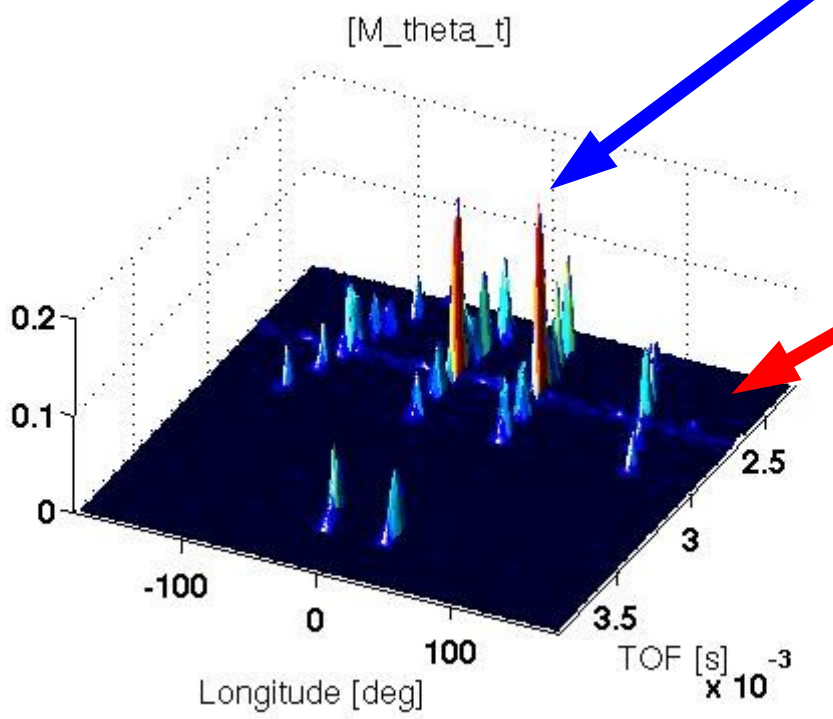
- Focus virtual experiment
- Cryo-furnace+*l*-Rb



Quantitative estimate of instrument effects (resolution, beam distributions, ...)

Focus@PSI : Resolution function

Idea (N. Takahashi): use a Dirac brush



Each Dirac scatters a **resolution function**

Incoherent line

You can do it !

To perform similar studies you need:

- to use McStas
- to describe your instrument setup
- to describe the sample environment
- to know the sample S(q,ω)

S(q,ω) may come from:

- Molecular Dynamics/ab initio simulations
- analytical model
- previous experiments, with accurate data analysis (largest q,w range)

If you start such virtual experiments, send us your S(q,w) !!!