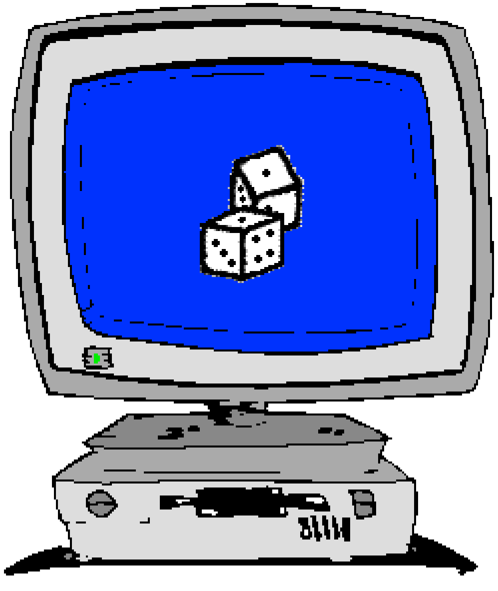
An introduction to

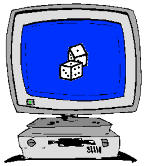
Neutron Scattering
Monte Carlo Ray-Tracing Methods
For Virtual Experiments

by E. Farhi, ILL/DS/CS



Outline

1. Definition of Monte Carlo methods
2. What for (in neutron scattering world) ?
3. The *McStas* neutron ray-tracing package
4. A few examples...
5. Do it yourself: how to...



Origin of Monte Carlo methods

Used by Nature since ... (a long time) : diversity of Life

First application using computers:

Metropolis, Ulam and Von Neumann at Los Alamos, 1943

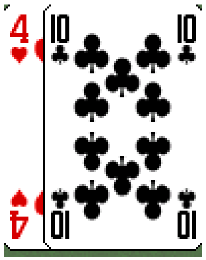
Neutron Scattering and Absorption in *U* and *Pu*, Origin of *MCNP*

Name:

Monte Carlo Casino, a random generator (Ulam played poker)

Photograph Source: GALE FORCE Archive

What are Monte Carlo methods ?



- Use random generators (play poker)
- Explore a complex and large phase space (many parameters)
- Integrates microscopic random events into measurable quantities
  not a usual regular sampling integration

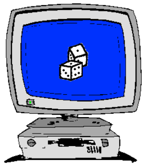
$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1, a<u_i<b}^{n} f(u_i) = \frac{1}{b-a} \int_a^b f(u)\, du$$

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

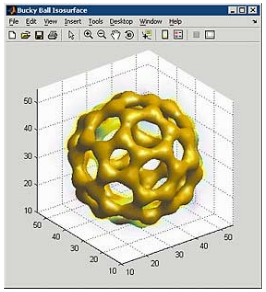
$$p \ \alpha \ e^{-E/kT}$$

- 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.



When to use Monte Carlo methods



Dimensionality of phase space must be large ($d > 5$)

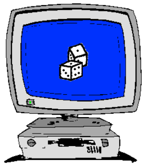
Overall complexity is beyond reasonable analytical methods

Each event can be computed easily and independently

MC is the '*lazy guy*' method – think microscopic

Examples:

- Molecular Dynamics
- spin-system phase transitions (*Ising* model)
- nuclear reactions
- ray-tracing (light, particles)



Some Monte Carlo programs

Light ray-tracing: PoV-RAY and others ...

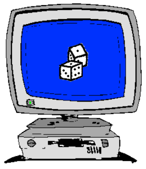
Nuclear reactor simulations (neutron transport):
MCNP, Tripoli, GEANT4, FLUKA

Neutron Ray-Tracing propagation:

- **McStas**

Neutrons are described as **(r, *v*, *s*, *t*)**, and are transported along models.

Each time physics takes place (scattering, absorption, ...) random choices are made. Propagation simply use Newton rules, *incl*. gravitation.



How to implement Monte Carlo methods ?

Good random generator:

- from thermal electronic noise (hardware)
- or quasi-random generators **=>** *quasi*-Monte-Carlo

We shot *n* events, we encounter a probability $\mathbf{0 < p < 1}$.

Crude Monte-Carlo (yes/no choice):

Keep only *np* events

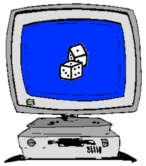
Low statistics

Importance sampling (fuzzy choice – event weightening):

Keep *n* events

But associate a **weight** *p* to each of them

Retain statistical accuracy ($1/\sqrt{n}$)

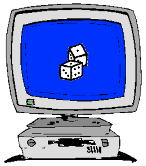


Why simulate neutron instruments+samples ?

- Design new instruments
- Optimize existing instruments (flux/resolution)
- Optimize usage of existing instruments (better experiments)
- **Get accustomed with the instruments before coming at the ILL**
- Measure the instrument effects on the simulated 'ideal' sample signal
- Estimate complex effects like :

    absorption, multiple scattering, geometry, resolution function...

- Compare virtual experiments with real ones, possibly during exp.



Virtual experiments

Virtual experiments

=

Instrument simulation

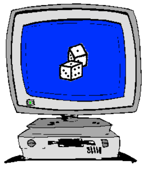
⊗

Realistic Sample model

=

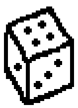
Neutron *flight simulator*

and then we play with it without breaking the instrument and sample



Presentation of *McStas*

Flexible, general simulation utility for neutron scattering experiments.



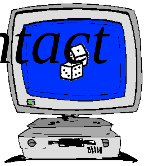
Original design for *M*onte *C*arlo *S*imulation of *t*riple *a*xis *s*pectrometers.
Developed at RISØ and ILL (started 1998).
Mainly funded by EU (FP 4-7): 2.5+1 people full time, plus projects.
Open source, GPL2. Works on all systems, binaries for *Linux*, *Win$*, *MacOSX*

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

Probably a few hundred users worldwide (200 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*



A bit of theory for neutron-sample interaction

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

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

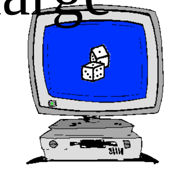
Probability to interact

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

Scattering distribution

$S(q,\omega)$

with importance sampling to scatter preferably where *S* is large



Liquid Indium real and virtual experiment

Liquid Indium:

- Very low scattering cross section (*good luck*)
- Very high absorption (*good luck*)
- Never measured with neutrons (*good luck*)

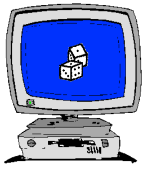
Proposal includes both real and virtual experiment:

Simulation showed we would be able to measure the quasi-elastic line
Around the first structure peak in *S(q)*.

Experiment:

Levitation furnace (gas flow+laser)
T=450 K
IN22 Ei=30.8 meV

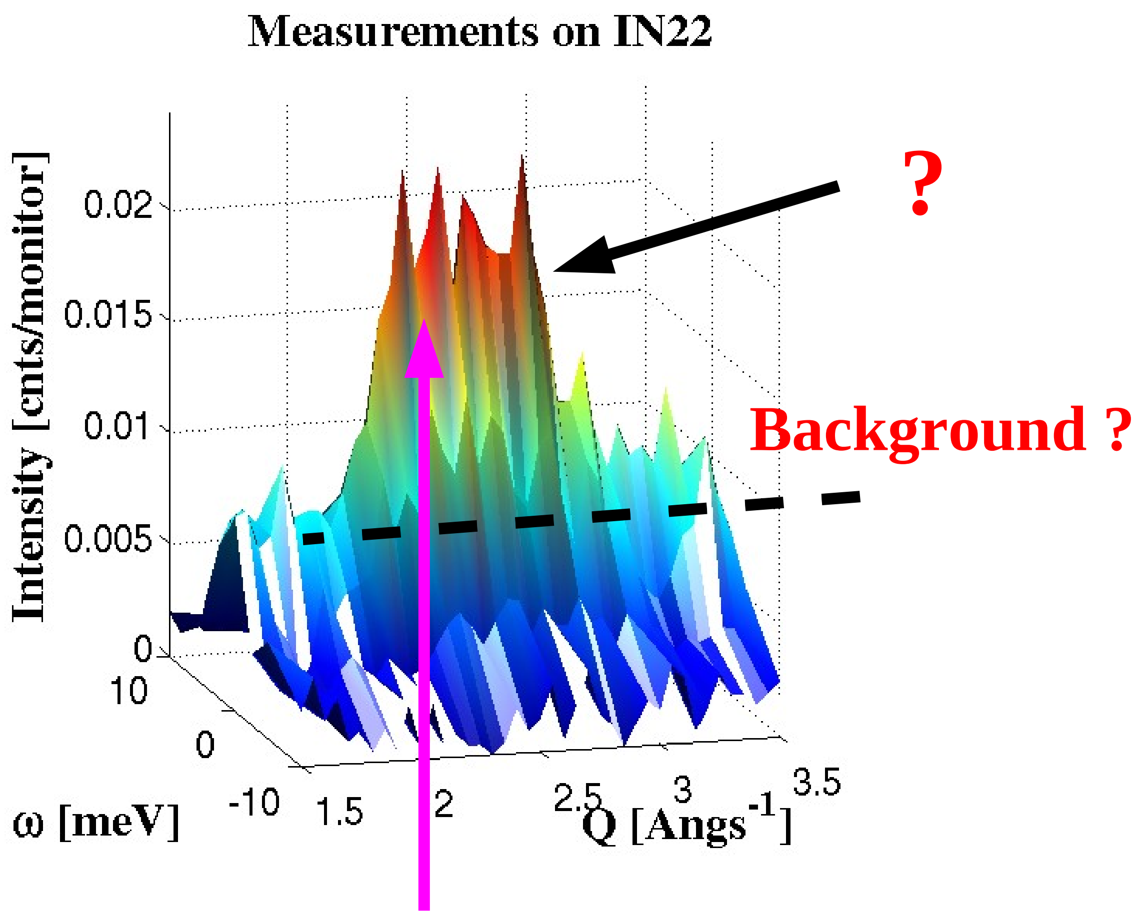
Team: E. Farhi, P. Willendrup, L.P.Regnault, McStas <mcstas.org>

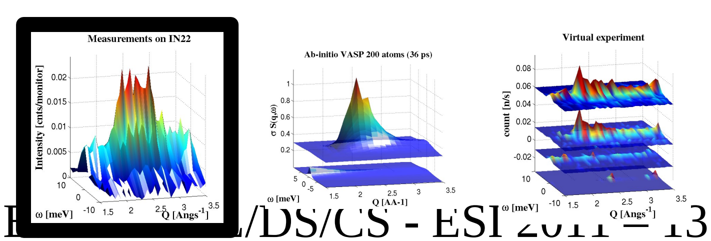


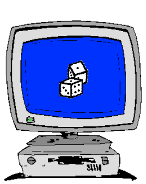
Liquid Indium real experiment

Data includes contribution from the furnace and the B4C nozzle.
Sample is a ϕ=4mm diameter sphere

Experiment produces...





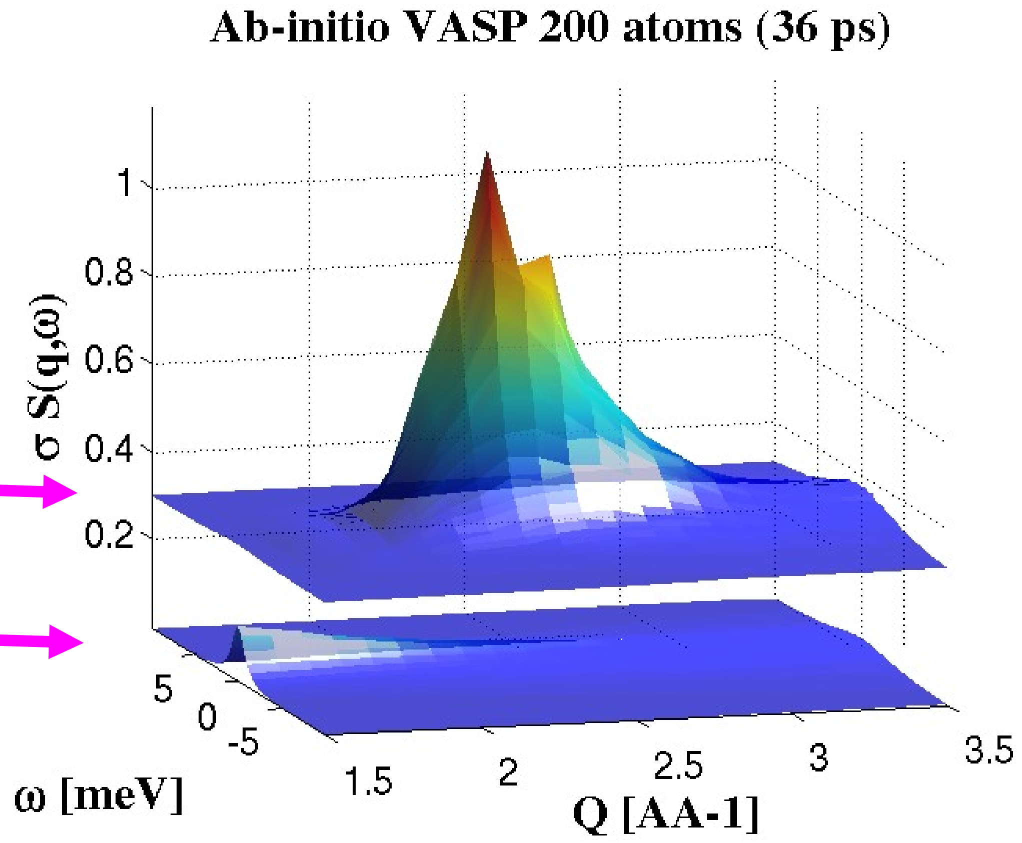


Liquid Indium: Ab-Initio Molecular Dynamics

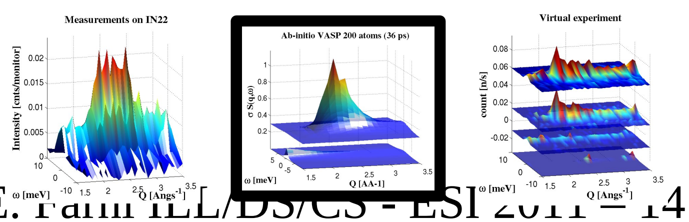
We use *VASP*
200 atoms in a 17 Å cube
Record atoms dynamics for 36 ps
Compute *S(q,ω)* using *nMoldyn*

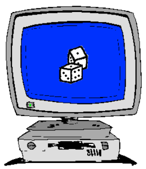
Coherent part

Incoherent part



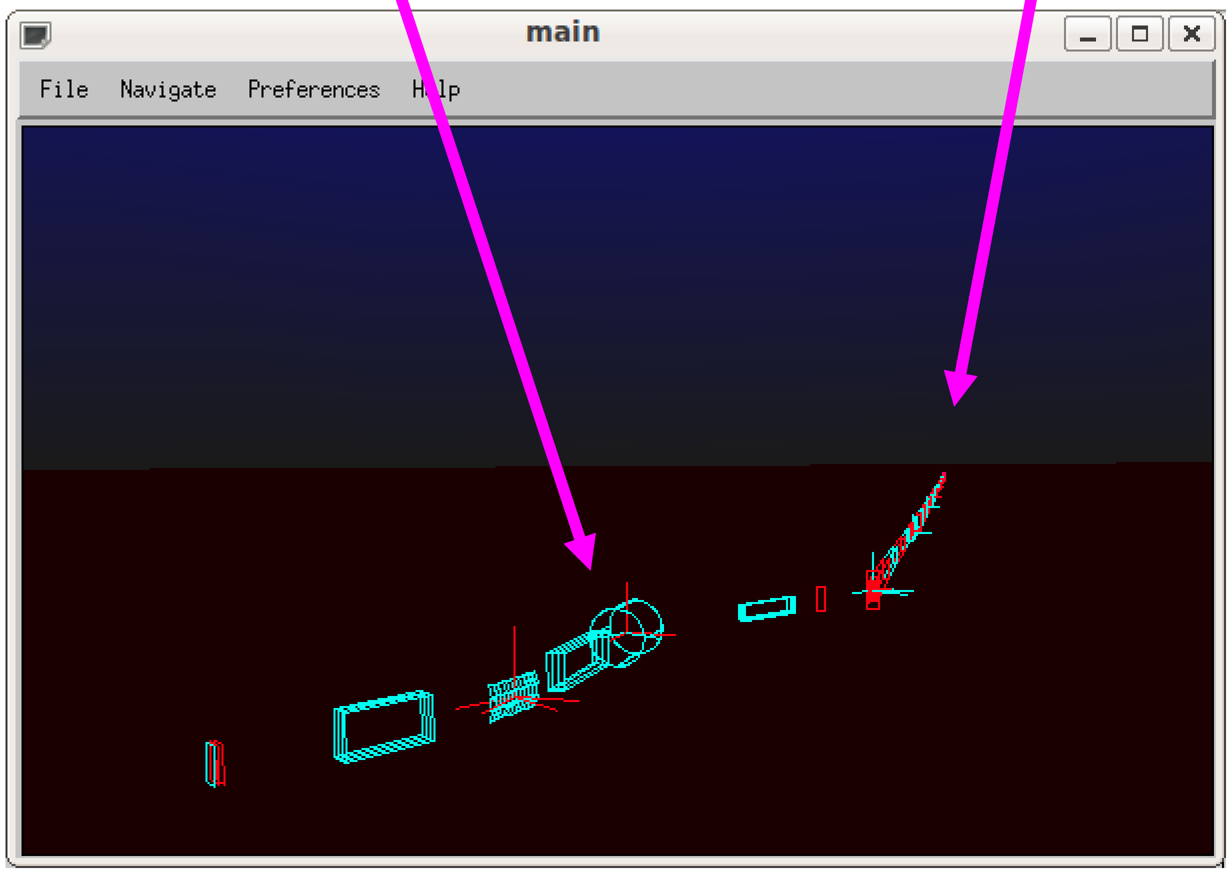
We show here the measurement range
Compared to experiment,
computed S(q,ω) is very clean

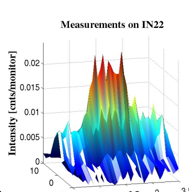


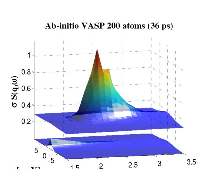


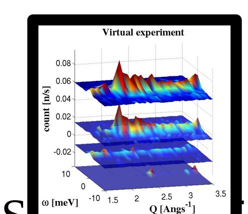
Liquid Indium: Virtual experiment

We use *McStas* <mcstas.org> to model the reactor, the H25 supermirror Guide and the IN22 triple-axis spectrometer.
Model includes levitation furnace and nozzle.

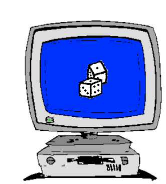




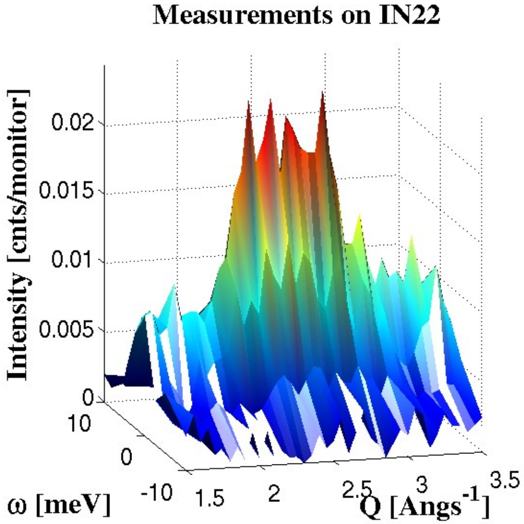


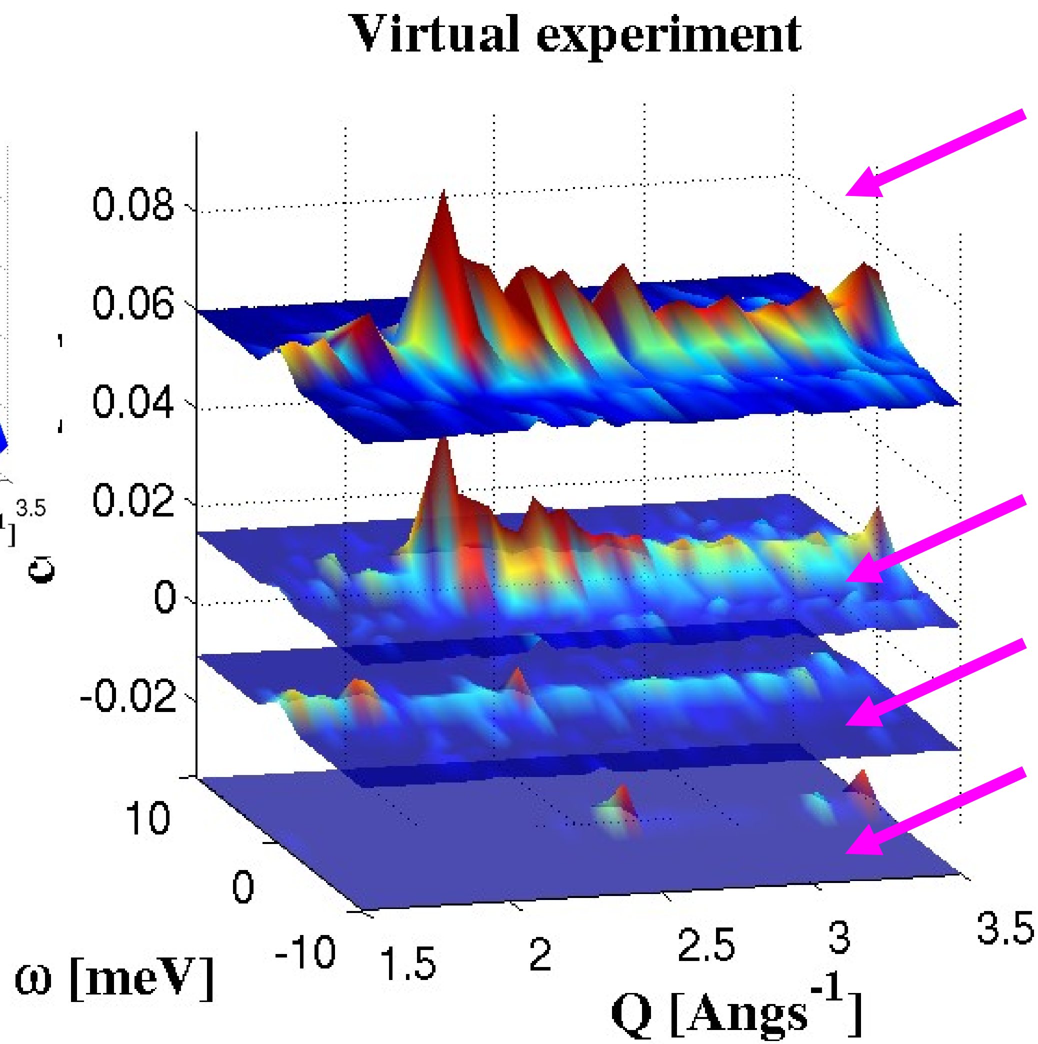


We run on 80 cores for 4 hours to simulate all *q*-energy scans.



Liquid Indium: Virtual experiment (cont'd)



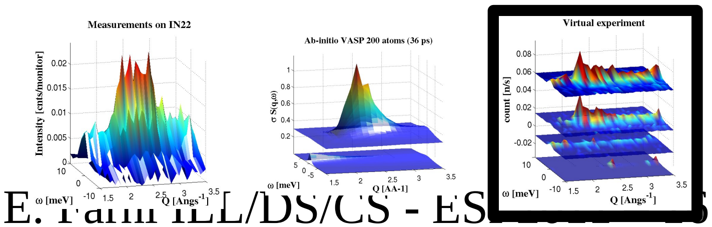


Total signal shows a tail after the structure peak

Coherent part

Incoherent part

Furnace contribution



Virtual experiment enables to **prepare and understand** the measurement.

***l*-In measured with neutron**