# Simulating neutron instruments and experiments

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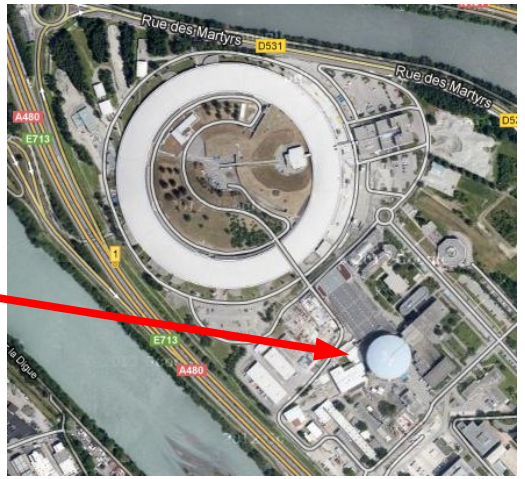



Staff: 400
Exp./y: 1100+
~30 instruments

# ~~~ The Menu ~~~

- What is Monte-Carlo ? (not only a casino)
- Instrument simulation codes
- Instrument components
- Examples of neutron instruments
- Virtual experiments
- Demo: a diffractometer, TAS, a UCN moderator

# 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

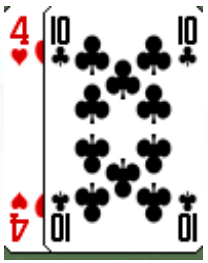
Neutron Scattering and Absorption in *U* and *Pu*, Origin of *MCNP*

**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

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

- Integrals converge faster than *any* other method (for $d > 3$)

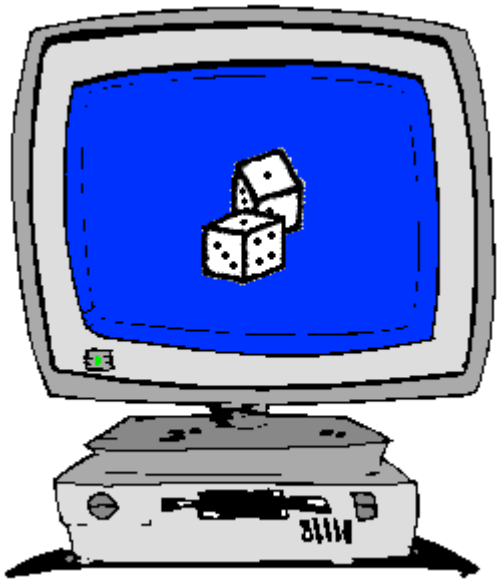
  when using *enough* independent events (central limit theorem)

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

# *How to implement Monte Carlo methods ?*

**Good random generator**:

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



We encounter a probability $0 < p < 1$.

**Crude Monte-Carlo** (yes/no choice):

We shoot $n$ events $\xi \in [0,1]$

We keep events that satisfy $\xi < p$

$np$ events → low statistics

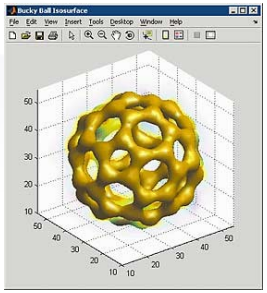
**Importance sampling (fuzzy choice – event weighting)**:

Keep $n$ events, no more random number...

But associate a **weight** $p$ to each of them (we set $\xi = p$)

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

# When to use Monte Carlo methods



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

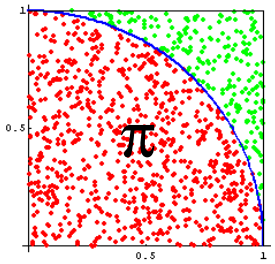
Overall complexity is beyond reasonable analytical methods

Each event can be computed easily and independently

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

**Examples:**

- Estimate π from a circle/square ("*Buffon needle*")
- Area under/inside a curve/volume (integration)
- Molecular Dynamics
- spin-system phase transitions (*Ising* model)
- nuclear reactions
- ray-tracing (light, particles)




Number of points for which
$\{ x^2+y^2 \leq 1, (x,y) \in [0,1] \}$
Ratio circle/square → $\pi/4$

# *Some Monte Carlo programs*

***Each time physics takes place (scattering, absorption, ...) random choices are made.***

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

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

Neutron Ray-Tracing propagation:
**McStas <www.mcstas.org>**, Vitess, Restrax, NISP, IDEAS
*Neutrons are described as **(r, v, s, t)**, and are transported along models.*
*Propagation simply uses Newton rules, incl. gravitation.*

X-ray tracing
Shadow, McXtrace

# McStas: an EU neutron scattering Monte-Carlo code

**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, source and binaries for *Linux, Win$, MacOSX, Live-DVD*

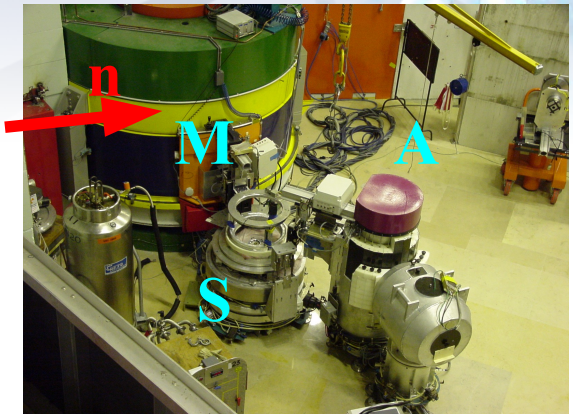
Most widely used code in its ecological niche (compared to other similar codes)..

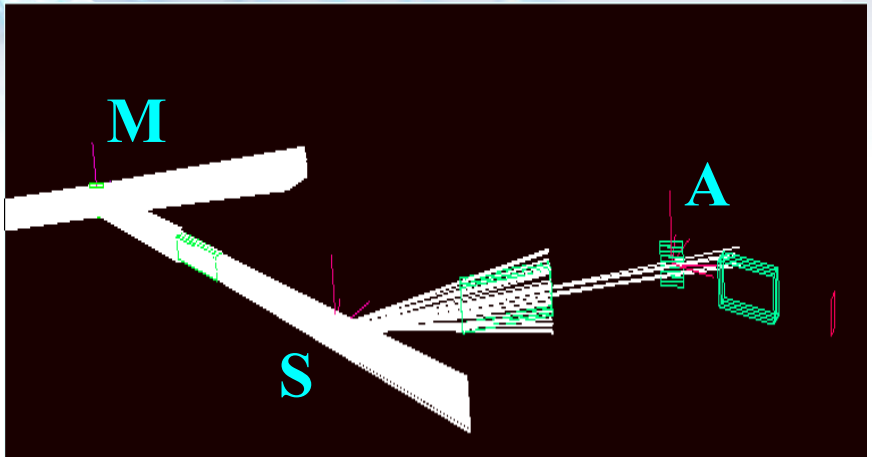
A few hundred users worldwide
some contributors (community based).
*Has been used to model most existing and future neutron scattering instruments.*

<www.mcstas.org>

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

# Simulating instrument: what for ?



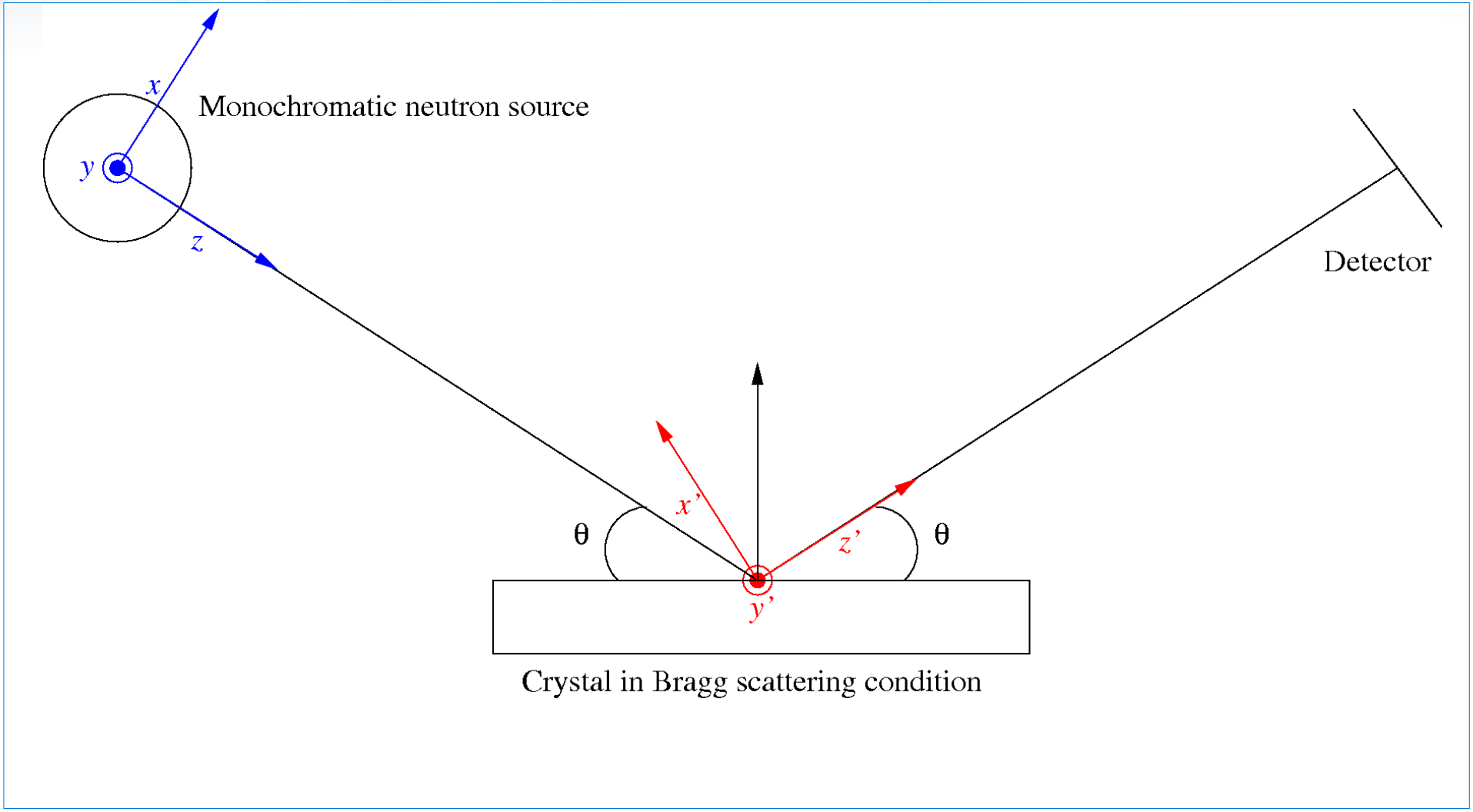

*A Triple-Axis Spectrometer (IN20)*

- 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.

# Schematic neutron propagation

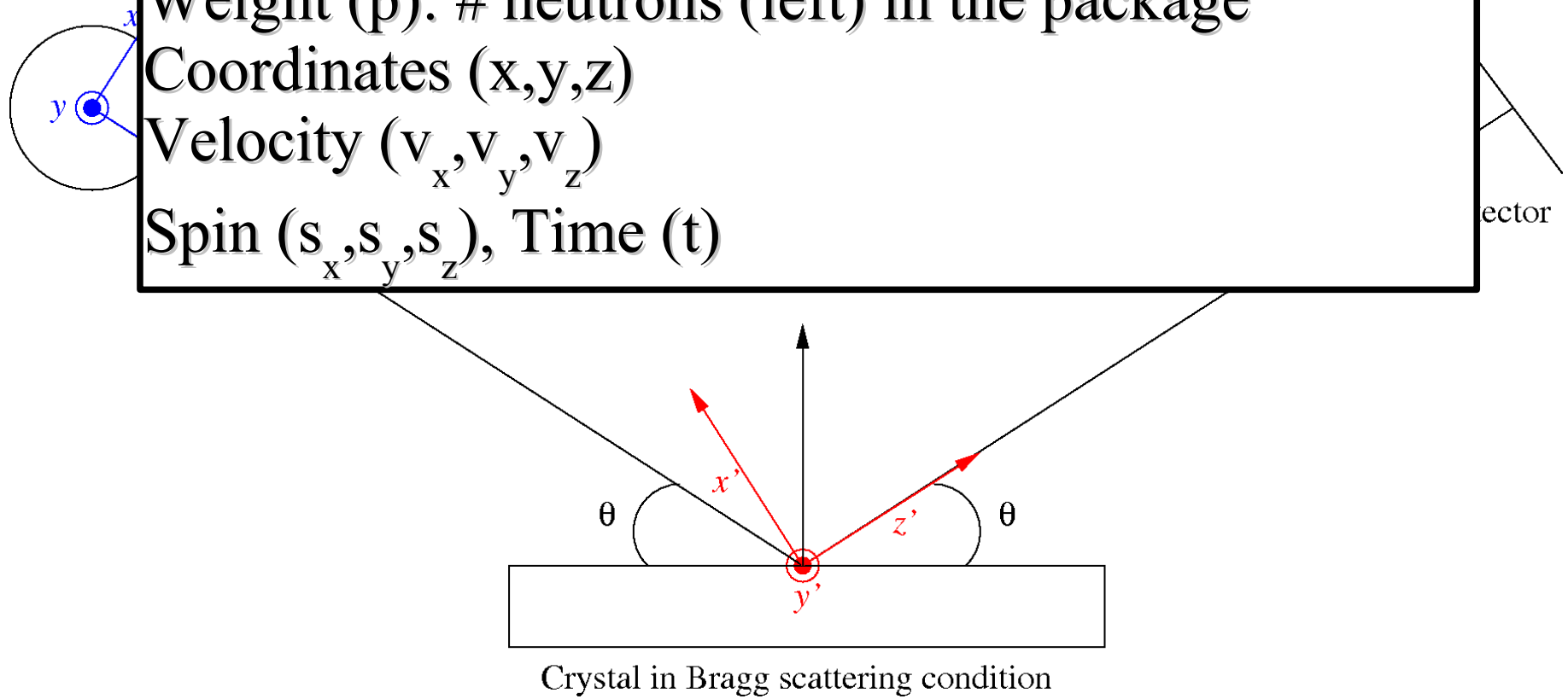


# Schematic neutron propagation

n

Neutron ray/package:

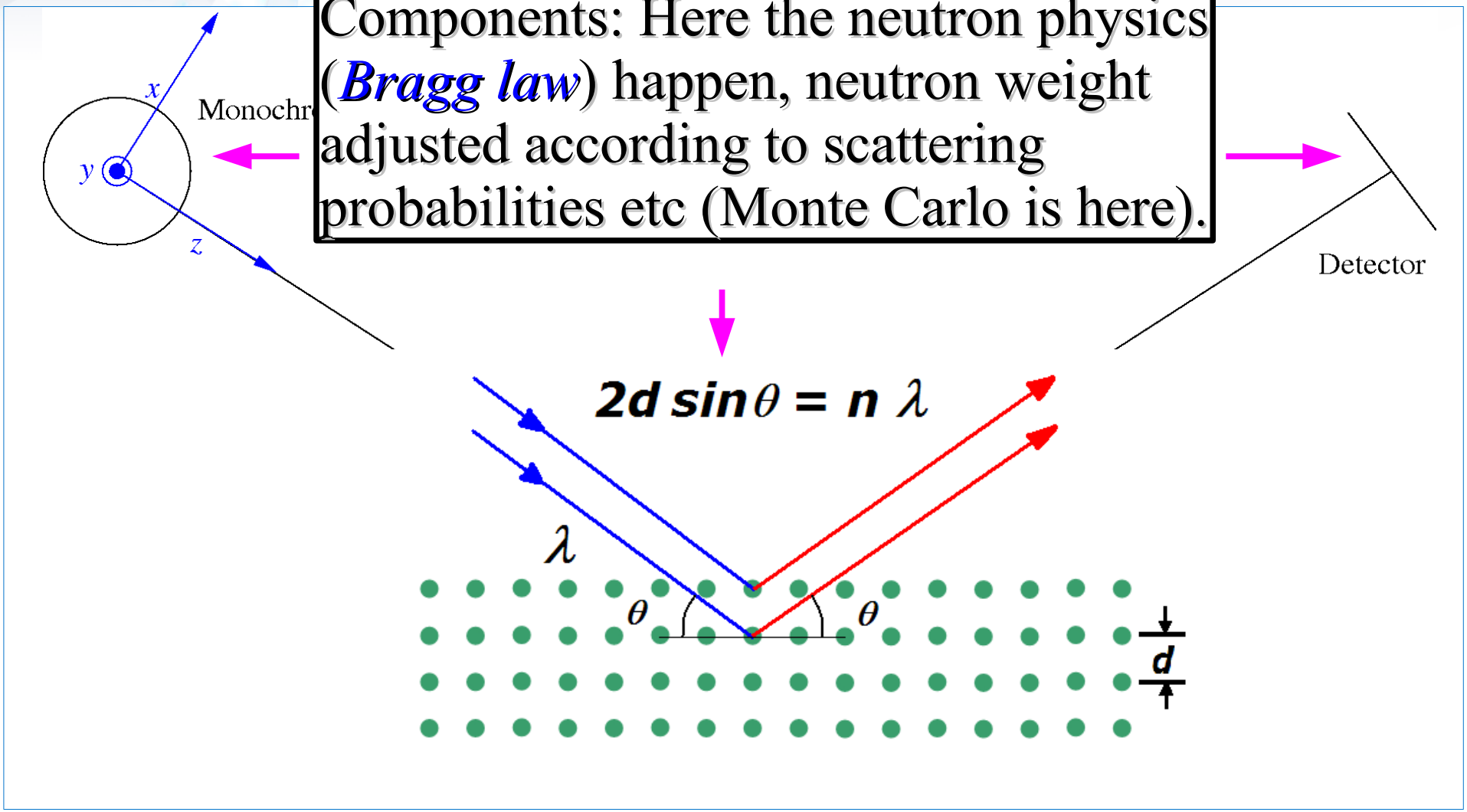
Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity ($v_x$,$v_y$,$v_z$)
Spin ($s_x$,$s_y$,$s_z$), Time (t)




Crystal in Bragg scattering condition

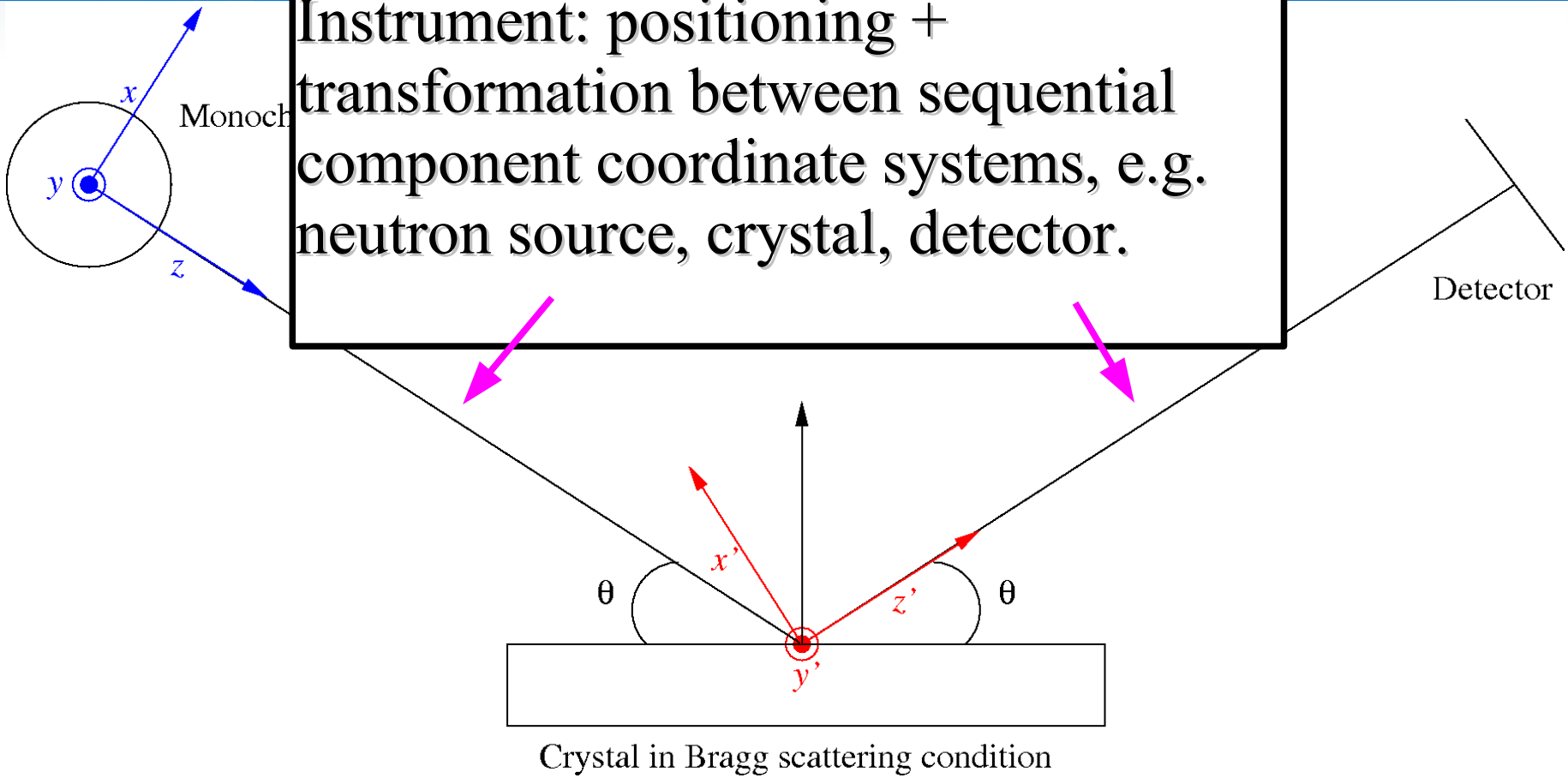
# Schematic neutron propagation

Components: Here the neutron physics (*Bragg law*) happen, neutron weight adjusted according to scattering probabilities etc (Monte Carlo is here).



# Schematic neutron propagation

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



# McStas grammar

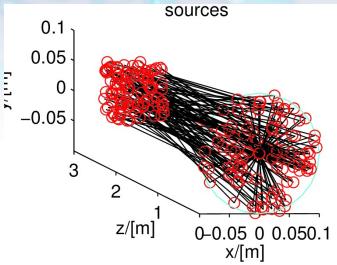
Instruments are defined from a text file. General syntax is based upon C.
Basic syntax:

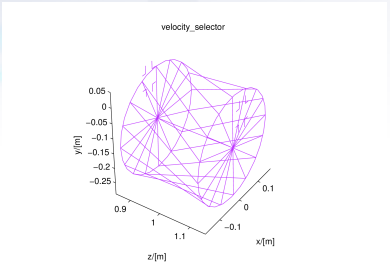
```
DEFINE INSTRUMENT name(parameter1=value1, …)

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
```

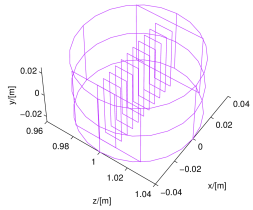
# McStas components

## Sources (neutrons)

Continuous (reactor), Pulsed

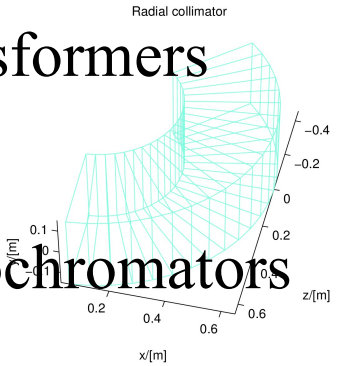


## Moving optics

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

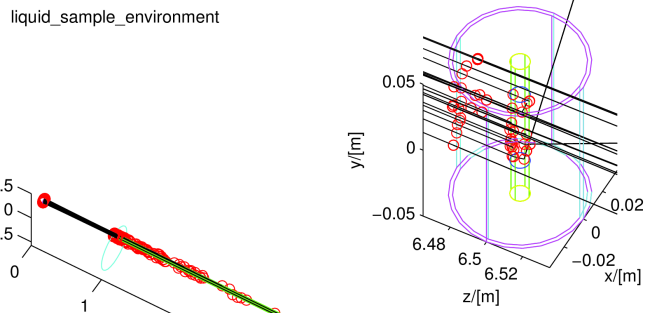



## Static optics

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

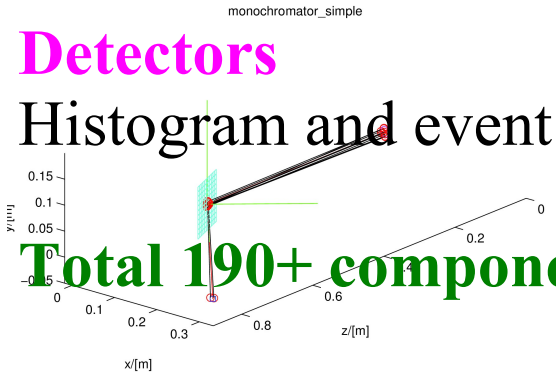
## Samples/materials

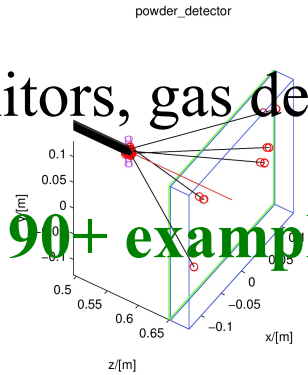
Single crystals, liquids, gas, polymers, hard spheres




## Detectors

Histogram and event monitors, gas detectors




**Total 190+ components, 90+ examples, manuals, tutorials...**

# *Virtual experiments: definition*

**Virtual experiments**

**=**

**Instrument simulation**

**⊗**

**Realistic Sample model**

**=**

**Neutron *flight simulator***

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


•E. Farhi *et al*, *J. of Comp. Phys.* **228** (2009) 5251
•E. Farhi and P. Willendrup, *Collection SFN* **12** (2011) 303
•E. Farhi *et al.*, *J. Neut. Res.*, **18** (2013)

# McStas: available sample components

Most instrument components are 'easy' to implement.
The samples are often more complex.

| *Scattering* | *Input* | *Coherent* | | *Incoherent* | | *Multiple* |
|---|---|---|---|---|---|---|
| *Process* | | *Elastic* | *Inelastic* | *Elastic* | *Inelastic* | |
| PowderN | $\|F^2(q)\|$,*abc*,$\sigma$ | Powder | | X | | |
| Single_crystal | $\|F^2(hkl)\|$,abc,$\sigma$ | Crystal | | X | | X |
| Isotropic_Sqw | S(q,w),$\sigma$ | Isotropic | X | X | X | X |
| Incoherent | $\sigma$ | | | X | QuasiE | |
| Sans_sphere | $\rho$,$\sigma$, $R$ | colloid | | | | |
| Sample_nxs | CIF data | Powder | | X | | X |

Sample geometry: box, cylinder, sphere, PLY/OFF file

# *Isotropic_Sqw: liquids, gas, glass, polymers, powders, …*

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** (1975) 1

We like to play games in $(q,\omega)$ 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 $(q,\omega)$ space

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

*Powder:*

$$\sigma_{\text{cone}} = \frac{V}{V_0^2}\frac{\lambda^3}{4\sin\theta}\sum_Q |F(Q)|^2$$

Probability to interact

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

Scattering distribution

$S(q,\omega)$

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

# Obtaining material characteristics

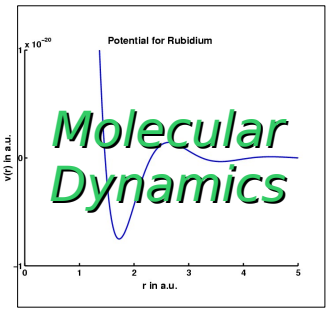
The dynamic structure factor $S(q,\omega)$ can be obtained from experiments, assuming a proper data reduction, or from MD.

*Experiments (TOF, TAS)*

*Detector efficiency, normalization, transmission (multiple scattering)*

**LAMP**
**FullProf**

$\theta \rightarrow q$ ; $t \rightarrow \omega$




*Molecular Dynamics*

**NAMD, DL_POLY**

Inter-atomic potential u(r)

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

*Ab-initio (VASP)*

Pseudo-potential

**VASP, CASTEP**

**R, v**

**nMoldyn**

.nc → .cdl → .sqw

**S(Q,ω)**
**S(Q)**
**F²(hkl)**

# *Benefits from a virtual experiment*

**Benefits:**

- The resolution from the instrument is implicitly convolved with the sample, without analytical integration
- The 'spurious' effects from the instrument can be included
- Treat absorption in the sample (self attenuation=2$^{nd}$ extinction)
- Treat coherent/incoherent scattering
- May include multiple scattering (depends on the sample component)
- May model the measurement background

**Requirements:**

- Need as accurate instrument description as possible
- Use proper sample component/kernel
- Give accurate data to the sample component (experiment, MD, …)
- Be critical regarding the results (*it's so easy to get rubbish*)

# *Time for examples*

1)A powder diffractometer

2)A triple axis: simulation and real (cool) stuff

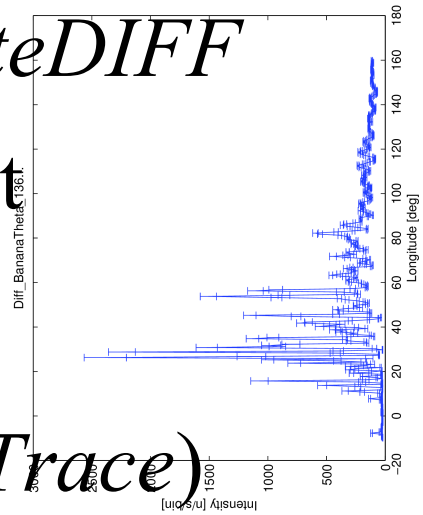
3)An advanced simulation of *very slow* neutrons

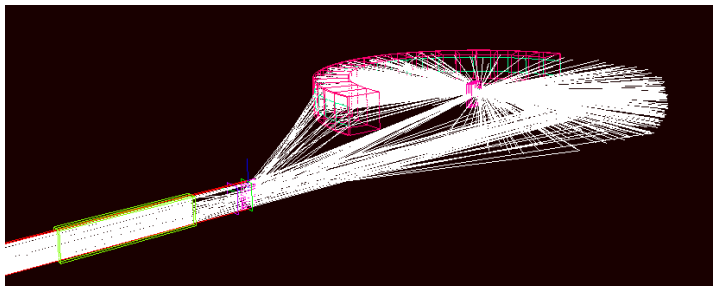
# Example 1: a powder diffractometer

- Crystallography represents about 30% (350/y) of the experiments.
- Allows accurate determination of composition and position of atoms in a material structure.
- Relies on Bragg law: $2d \sin \theta = n\lambda$
- Measures I($\theta$) for given $\lambda \rightarrow d \rightarrow$ atoms distances

# *Example 1: a powder diffractometer*

- Install McStas (here deb package)
- Launch McGUI/McStas
- Select *Neutron site* menu/*templates/templateDIFF*
- Click Run, then Start (with 2 cpu), then Plot
- Shows detectors in the simulation, and $I(\theta)$
- Re-run in 3D geometry view (*Simulate* → *Trace*)
- File can be exported in TXT, HDF, Matlab, (ROOT, MCNP/X) …
- Edit to see code



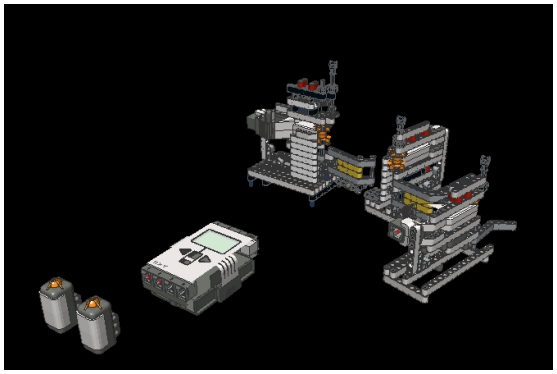



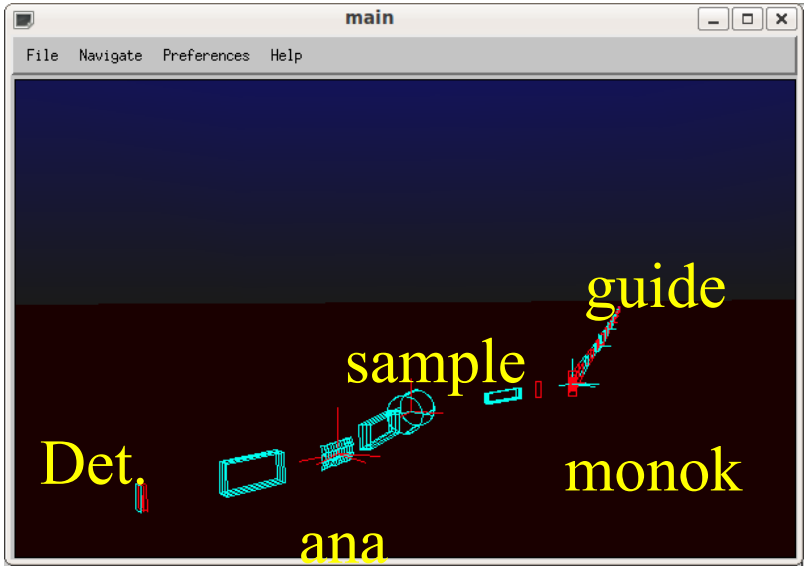
# Example 1: a powder diffractometer

- Estimate contribution from sample environment
- Notice it is removed by radial collimator
- Notice that gas detector has 65% efficiency at $\lambda$=1 Å

# Example 2: a triple-axis spectrometer

- We here use a modified version of IN8@ILL
- Includes an interface with LEGO NXT
- Positions the virtual, LEGO instrument (and real)
- (Real positioning is much slower – big robot)
- Let's try it.





# Example 2: TAS + liq-In

**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

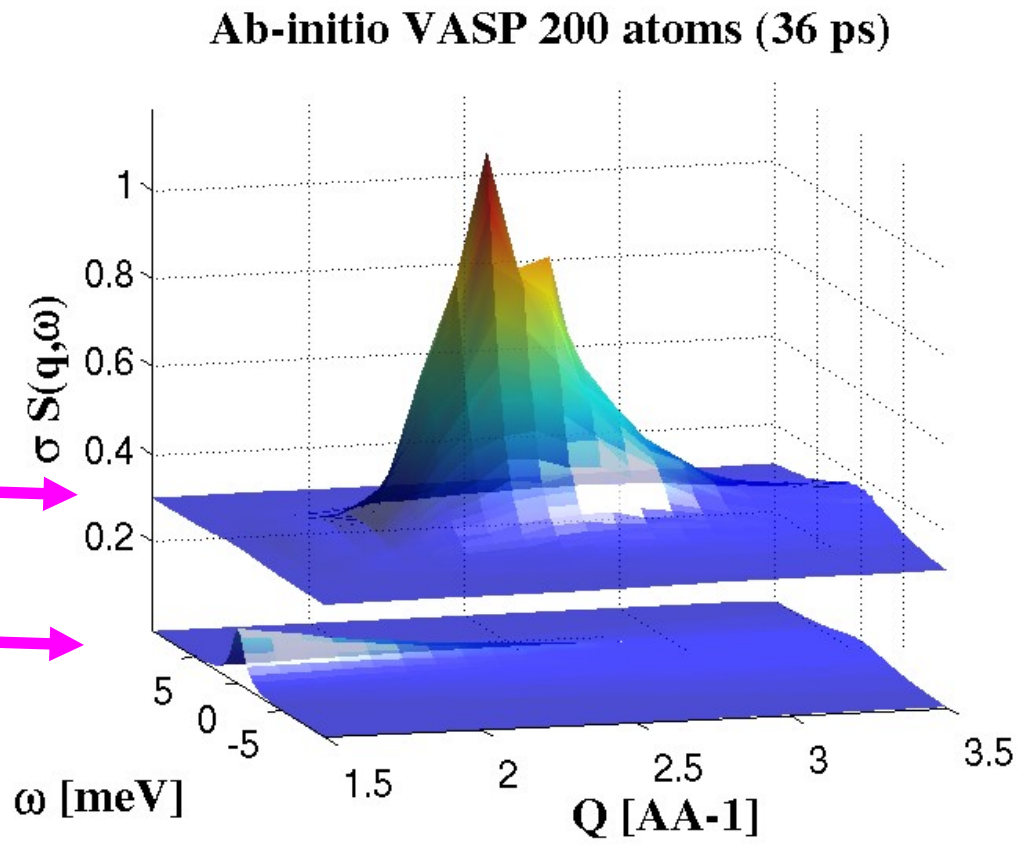
**Team:** E. Farhi, P. Willendrup, L.P.Regnault, McStas <mcstas.org>

# Example 2: TAS + liq-In: real world

# Example 2: TAS + liq-In

**Sample simulation**

We use *VASP (ab-initio MD)*
200 atoms in a 17 Å cube
Record atoms dynamics for 36 ps
Compute $S(q,\omega)$ using *nMoldyn*



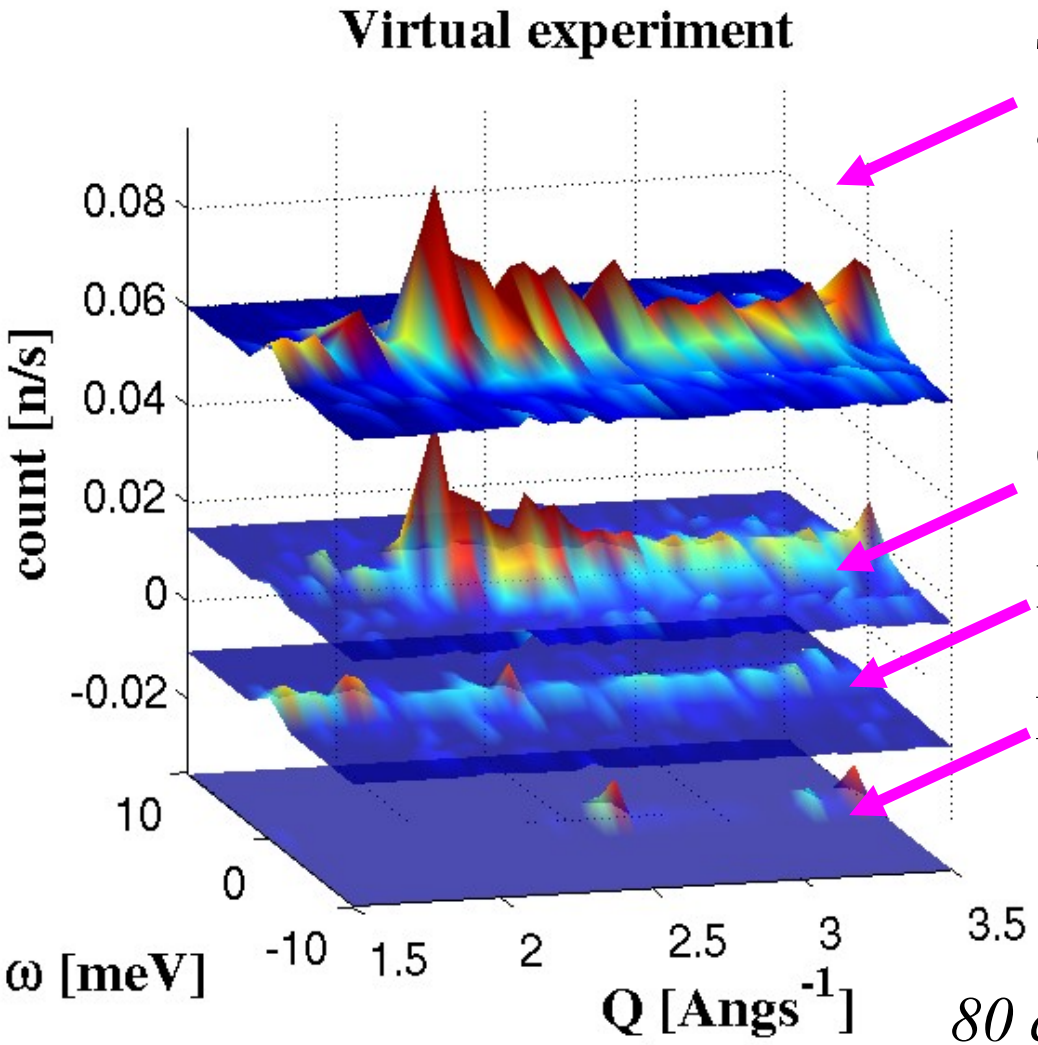

Coherent part

Incoherent part

*We show here the measurement range*
*Compared to experiment,*
*computed $S(q,\omega)$ is very clean*

# *Example 2: TAS + liq-In*

- Scanning momentum and energy exchange in the sample, we obtain the dynamic structure factor *S*.

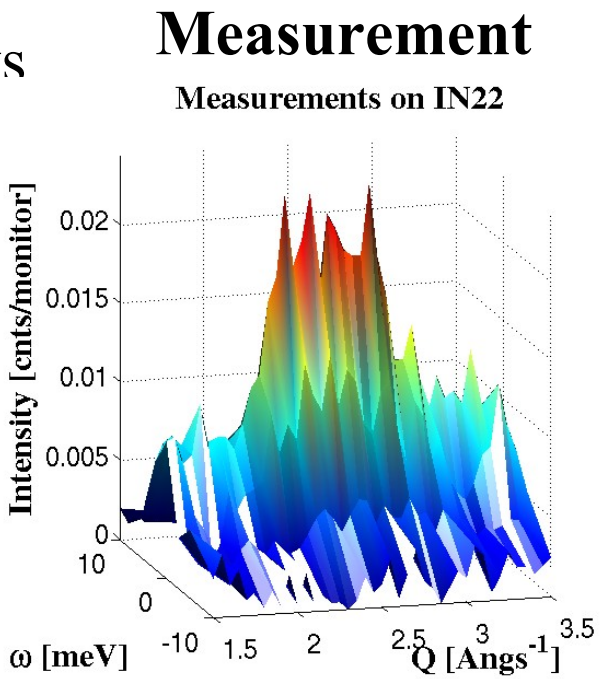



Total signal shows a tail after the structure peak

Coherent part

Incoherent part

Furnace contribution




*80 cpu, 4h*

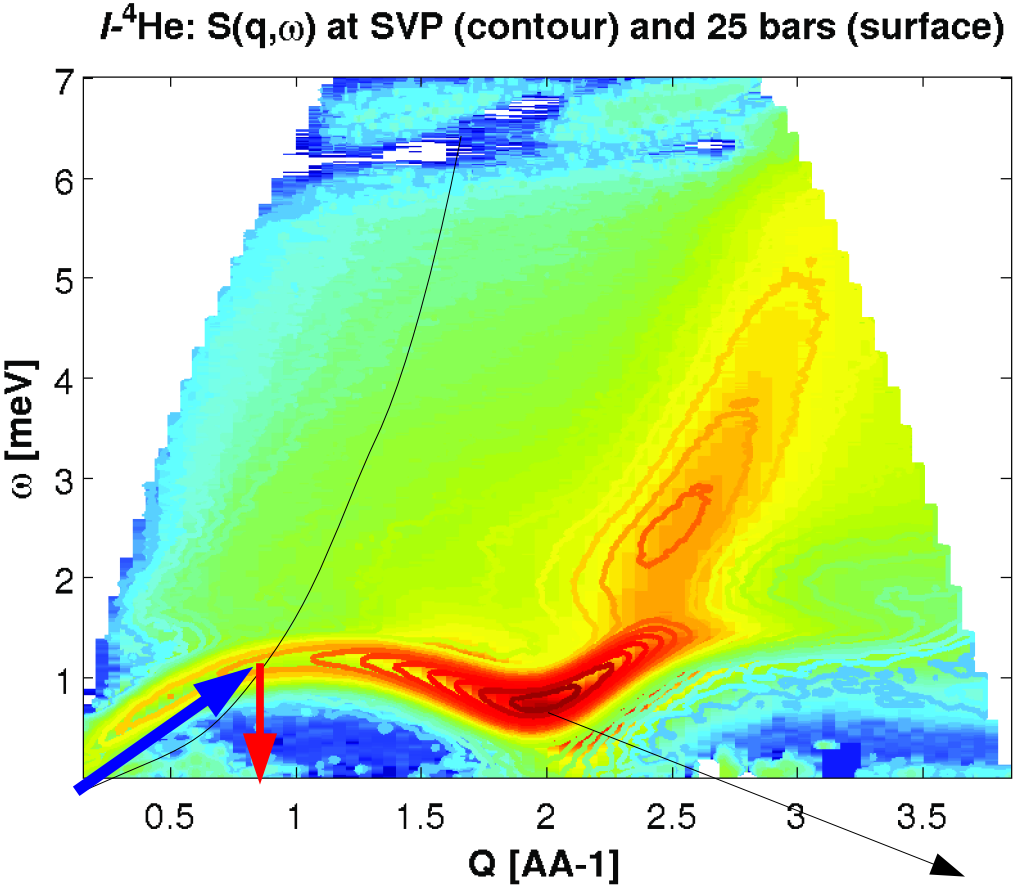
Virtual experiment enables to **prepare and understand** the measurement.

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

# Example 3: slowing neutrons ➞ 250 neV

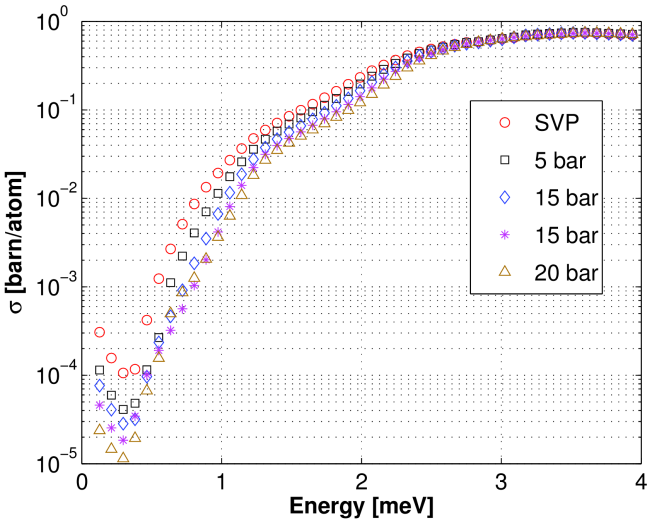
- Neutrons can give their energy to phonons in $^4$He

*Dynamic structure factor S*




$^4$He roton

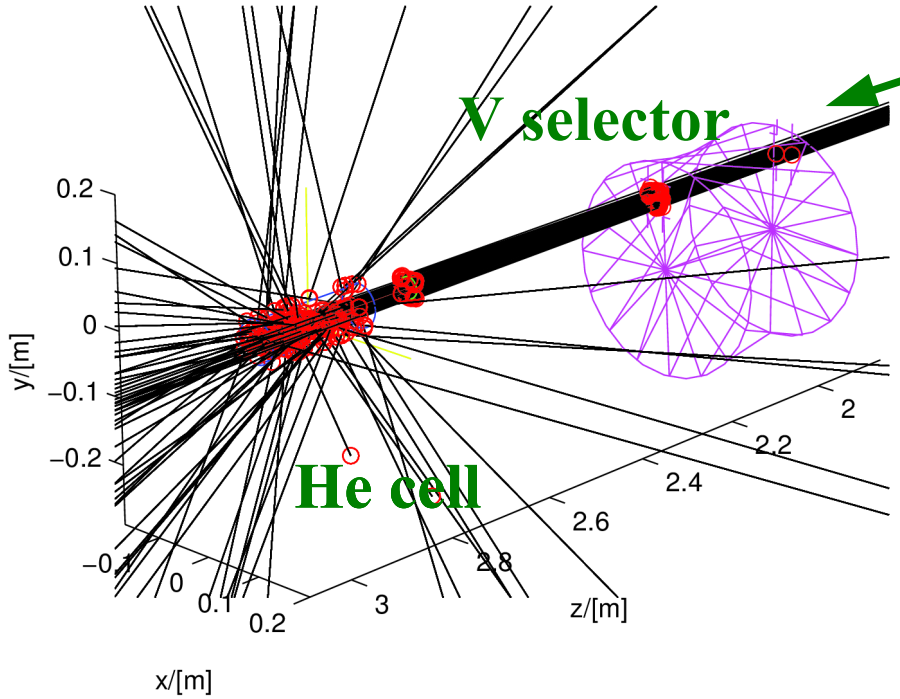
Total cross section



# Example 3: slowing neutrons ➞ 250 neV

Estimate how efficient the process is for creation of ultra-cold neutrons

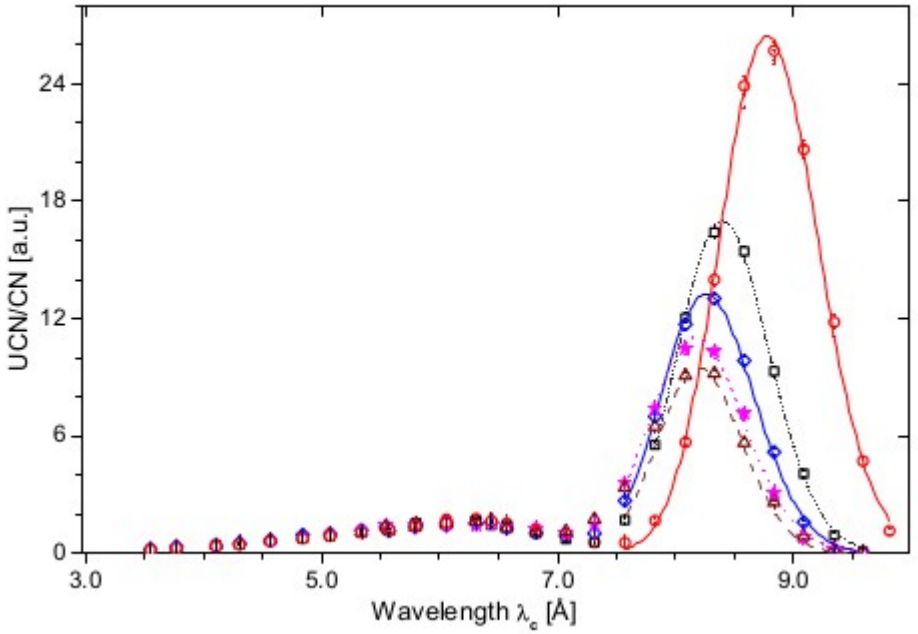
H113 guide@ILL



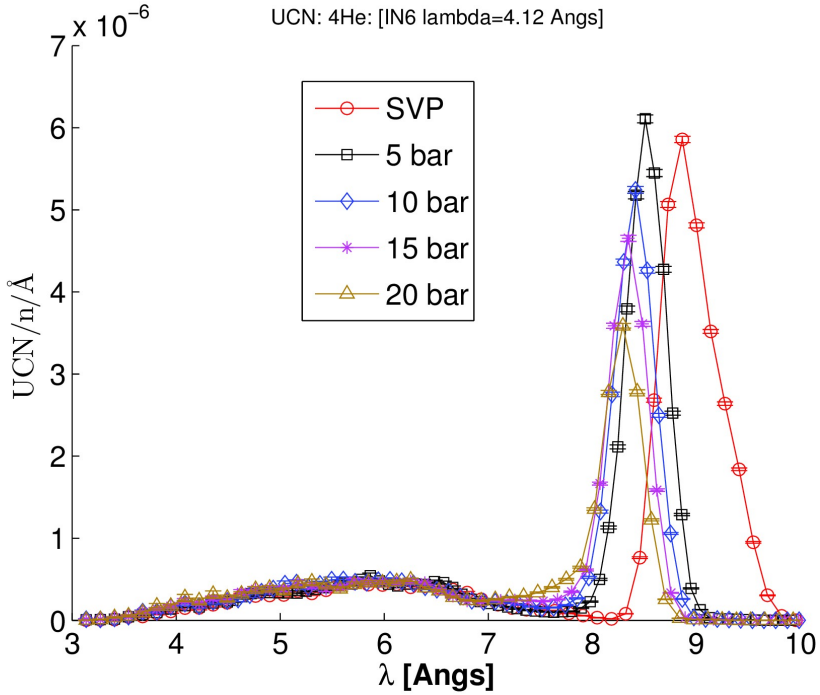

Start with 1-10 meV
Monitor <250 neV
Factor 4M loss

*96 cpu, 24h*

# Example 3: slowing neutrons ➡ 250 neV

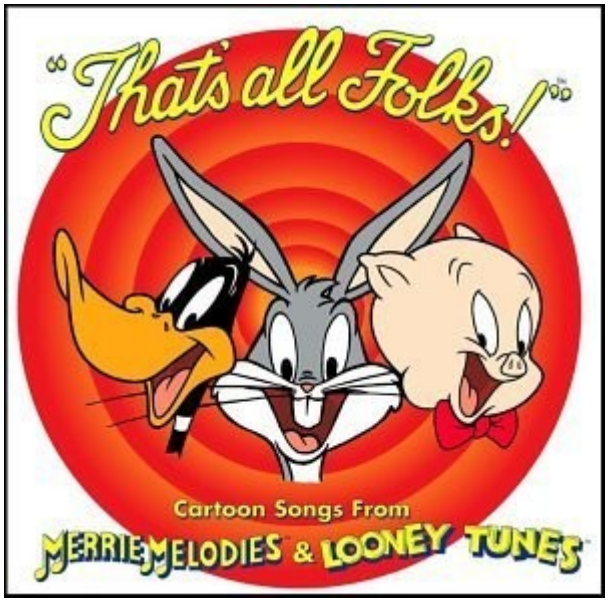



Measured




Simulated

Estimate how many UCN's can be generated at the ILL: up to **150-200**/cm3
Current world record **86** (ILL) with a mechanical Doppler turbine.


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