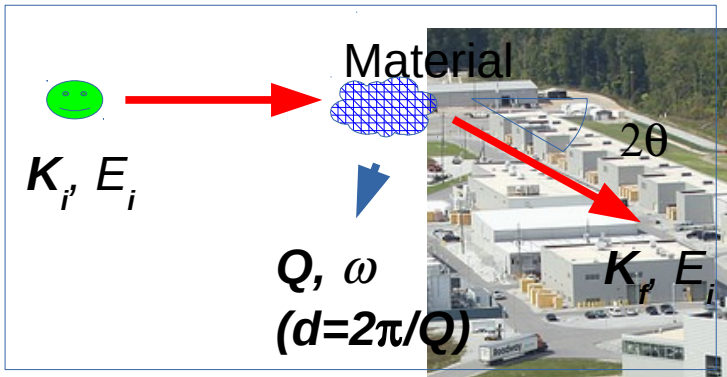
Neutron-matter interaction

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



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

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

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

Holy Book (Squires)

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

Dynamical structure factor *S(Q,ω)* is characteristic of each material
Reflects ordering of matter (atom/molecule positions – movements - domains)

Computing the total scattering probability

The total scattering cross section is given in (Ω,E_f) space, but *S* is given in (q,ω)
A variable change must be done for the integration (Jacobian).

We like to play games in (q,ω) space

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

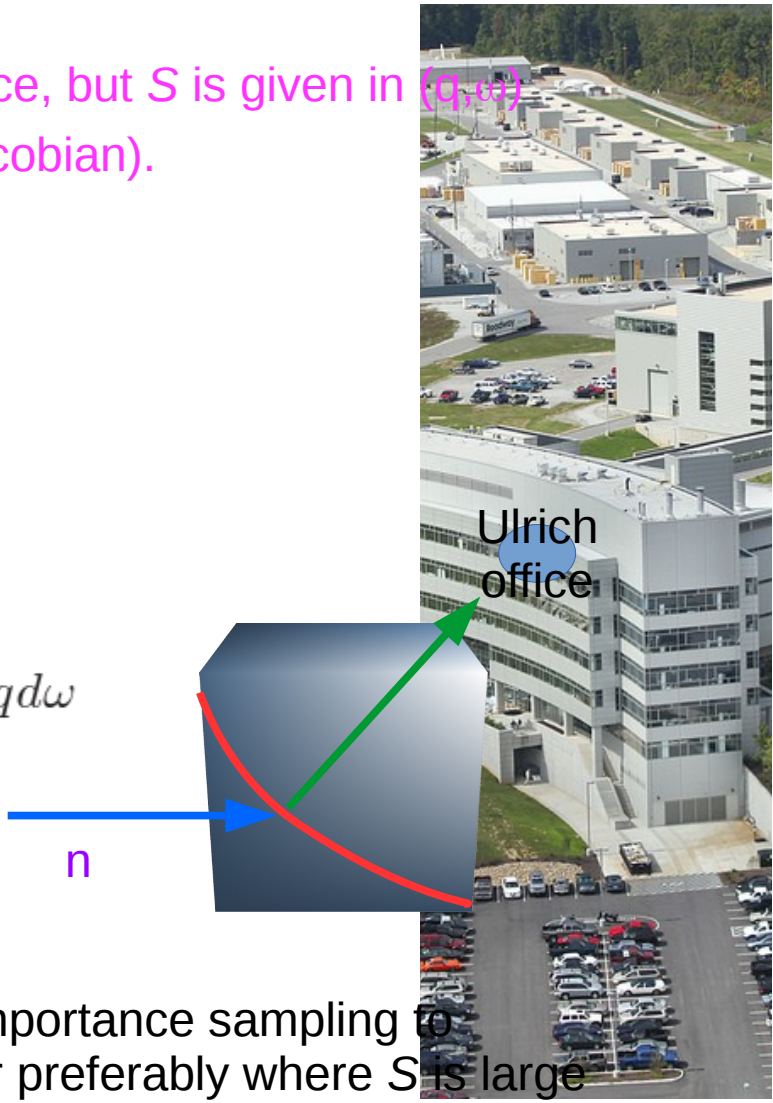
$$\frac{dq}{d\theta} = -\frac{k_i k_f sin\theta}{q}$$

Effective cross section in (q,ω) space

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

Probability to transmit

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



Scattering distribution

S(q,ω)

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

Isotropic_Sqw syntax

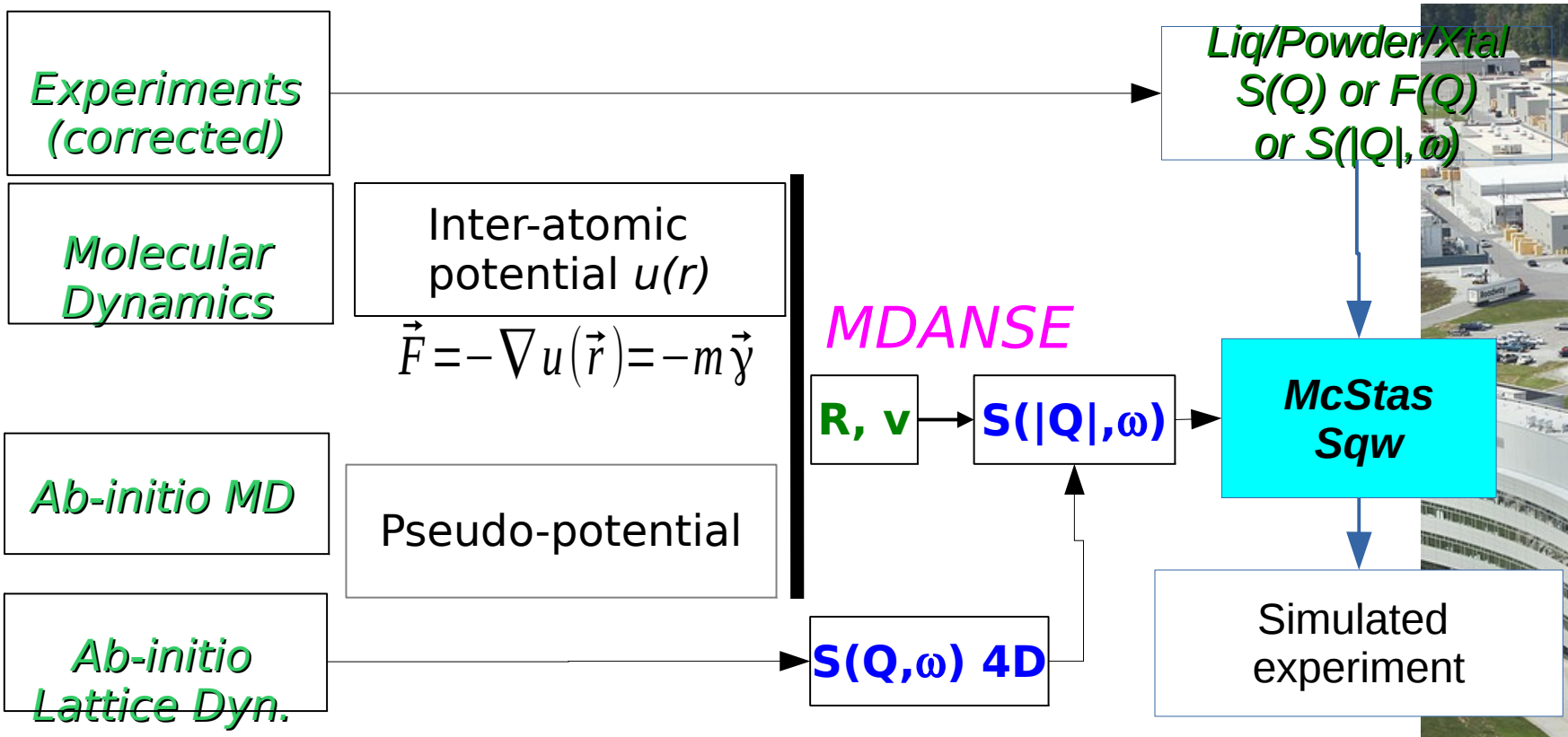
- ***Isotropic_Sqw(***
  Sqw_coh=FILE_COH,
  Sqw_inc=FILE_INC,
  radius=R,
  height=H)
- *More component parameters can specify geometry, physical properties, ...*
- *The data files specify the S(Q,ω) or S(Q) values as a matrix with Q,ω extent. Additional fields can be included as meta data (# lines).*

Isotropic_Sqw data format


```
# Sqw data file for Isotropic_Sqw
# liquid He4: coherent part, no incoherent, atomic number 2
# Elementary Excitation Data by R.J. Donnelly et al., J. Low Temp. Phys., 44 (1981) 471
# WARNING: line width is constant, intensity is not right
#
# Physical parameters:
# V_rho        0.072    atom density per Angs^3
# weight       4.002    in [g/mol]
# density      0.4784   in [g/cm^3]
# sigma_abs    0.00747 absorption scattering cross section in [barn]
# sigma_coh    1.34     coherent scattering cross section in [barn]
# sigma_inc    0        incoherent scattering cross section in [barn]
# Temperature 2         in [K]
# classical    0        experimental, contains Bose factor
#
# q axis values
# vector of m values in Angstroem-1
0.001000 0.011000 0.02 …
# w axis values
# vector of n values in meV
0.001391 0.011391 0.021391 0.0313 …
# sqw values (one line per q axis value)
# matrix of S(q,w) values (m rows x n values), one line per q value
9.721422 10.599145 11.344954  …
```

He4_liq_coh.sqw

How to get S(q,w) data sets



MD step is done prior to the virtual experiment (NAMD, VASP, GROMACS, ...). Computationally intensive (e.g. use clusters). Then use FFT(r,t)

McStas provides a few sample S(Q,w): Rb, Ge, H2O, D2O, D2, ...

Isotropic_Sqw: Handles **elastic** and **inelastic** for both **coherent** and **incoherent** channels

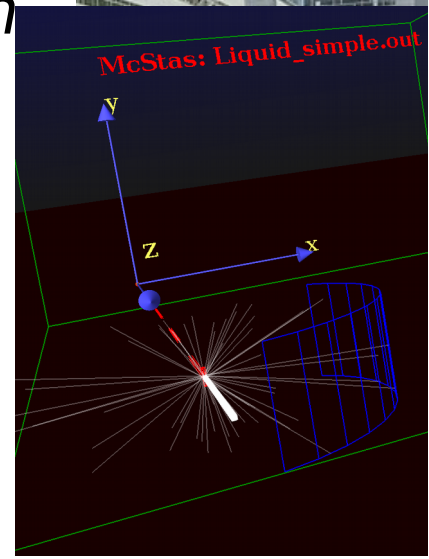
Sqw: a 'liquid' TOF

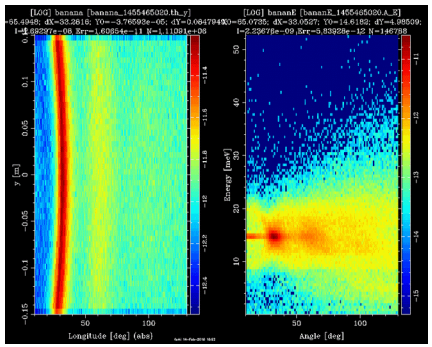
Aim: A simple spectrometer (and diffractometer)

- Create a new instrument from '*template (test)*'.
- Call it *Liquid_simple* and define input parameters `(lambda=2.36, string coh="Rb_liq_coh.sqw", string inc="Rb_liq_inc.sqw")`
- Insert a *Source_simple* ϕ1cm sending λ=lambda with $d\lambda/\lambda$=1%. Focus onto a 1x1cm^2 area.
- Insert an *Isotropic_Sqw* 3m away, using σ_{coh}=coh, σ_{inc}=inc with ϕ1cm x 5cm.

Sqw: a 'liquid' TOF

- Add a Monitor_nD cylindrical detector ϕ1m x 30cm, sensitive to **(θ,y)** for diffraction, centred on the sample, with 100 bins.
- Add the same, but sensitive to **(angle,energy)** with automatic energy limits.
- Save, run in Trace 3D to check geometry.
- Run in Simulation/PGPLOT mode with 1e8 neutron events.
- Plot results !
- Comment on the diffraction pattern and the inelastic one.





Sqw: a 'liquid' TOF: contributions

- *Insert an instrument variable in the DECLARE block, as 'flag_scat'.*

```
DECLARE %{

int flag_scat=0;

%}
```

- *After the AT token of the 'sample', insert an EXTEND block that sets flag_scat to the number of SCATTERED events.*

```
EXTEND %{

flag_scat=SCATTERED; // nb of scattered events

%}
```