

TOF spectrometer (direct geometry)



MDANSE 2018

**Simulation of Inelastic
Neutron Scattering
using McStas and
material dynamics models**

Sept. 24th – 28th 2018

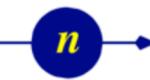
Puerto de la Cruz – Tenerife

(c) A. Martí (2012)

Useful links / docs

| <http://mcstas.org/links>

McStas



Overview of web resources for McStas

Get the code, report bugs etc.

- [McStas website](#)
- [McStas mailinglist subscription](#) (Please enrol!)
- [McStas Facebook page](#) (Please follow us!)
- [McStas downloads](#)
- [McStas+McXtrace GitHub](#)
- [McStas+McXtrace issues + bug reporting](#)

Neutron scattering + McStas e-learning

- [e-neutrons website](#) (free enrolment)

Tutorials, howto's, docs

- [How McStas works - in 2 minutes](#)
- [Tutorial: Build a SANS](#)
- [Tutorial: Build a diffractometer](#) (outdated in certain parts)
- [McStas user manual - Better use `mcdoc -m` in the terminal!](#)
- [McStas component manual - Better use `mcdoc -c` in the terminal!](#)
- [McStas component docs - Better use `mcdoc` in the terminal!](#)
- [McStas sample model functionality matrix](#) (not fully up to date)
- [McStas and McXtrace GitHub wiki - tutorials, guides and more](#)

| <https://github.com/McStasMcXtrace/McCode/wiki>

Documentation on the McCode tools

- [User documentation for the 2017- Python tool set](#)
- [mcrun variants - table overview](#)
- [mcplot variants - table overview](#)
- [mcdisplay variants - table overview](#)

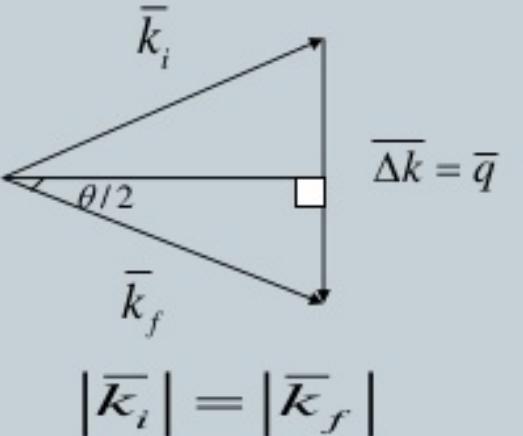




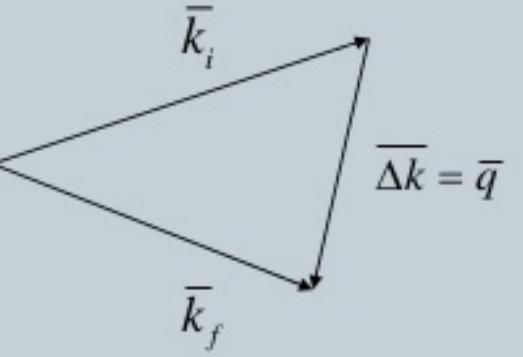
Spectroscopy reminder

TYPES OF SCATTERING

○

ELASTIC SCATTERING


$$|\bar{k}_i| = |\bar{k}_f|$$

INELASTIC SCATTERING


$$|\bar{k}_i| \neq |\bar{k}_f|$$

$$q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$

$$S(q) = \frac{d\sigma}{d\Omega}$$

Used to study structures

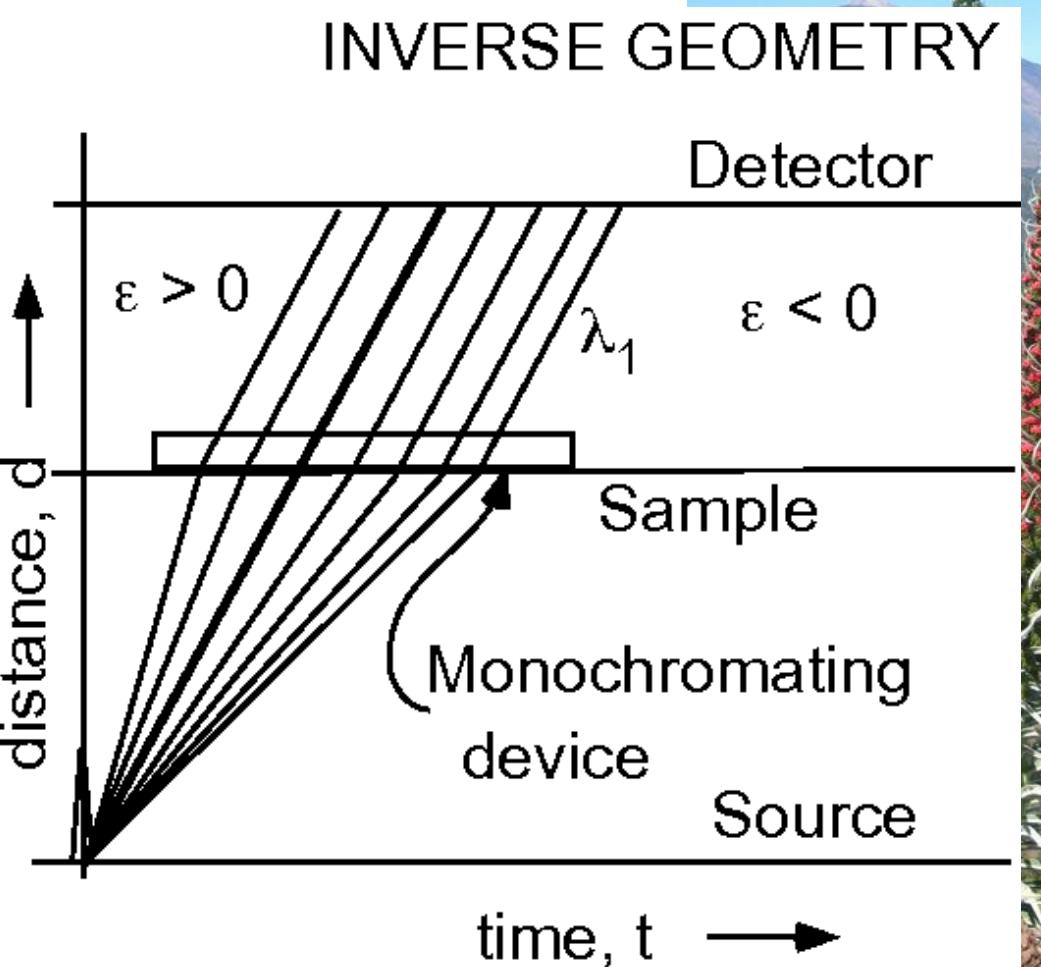
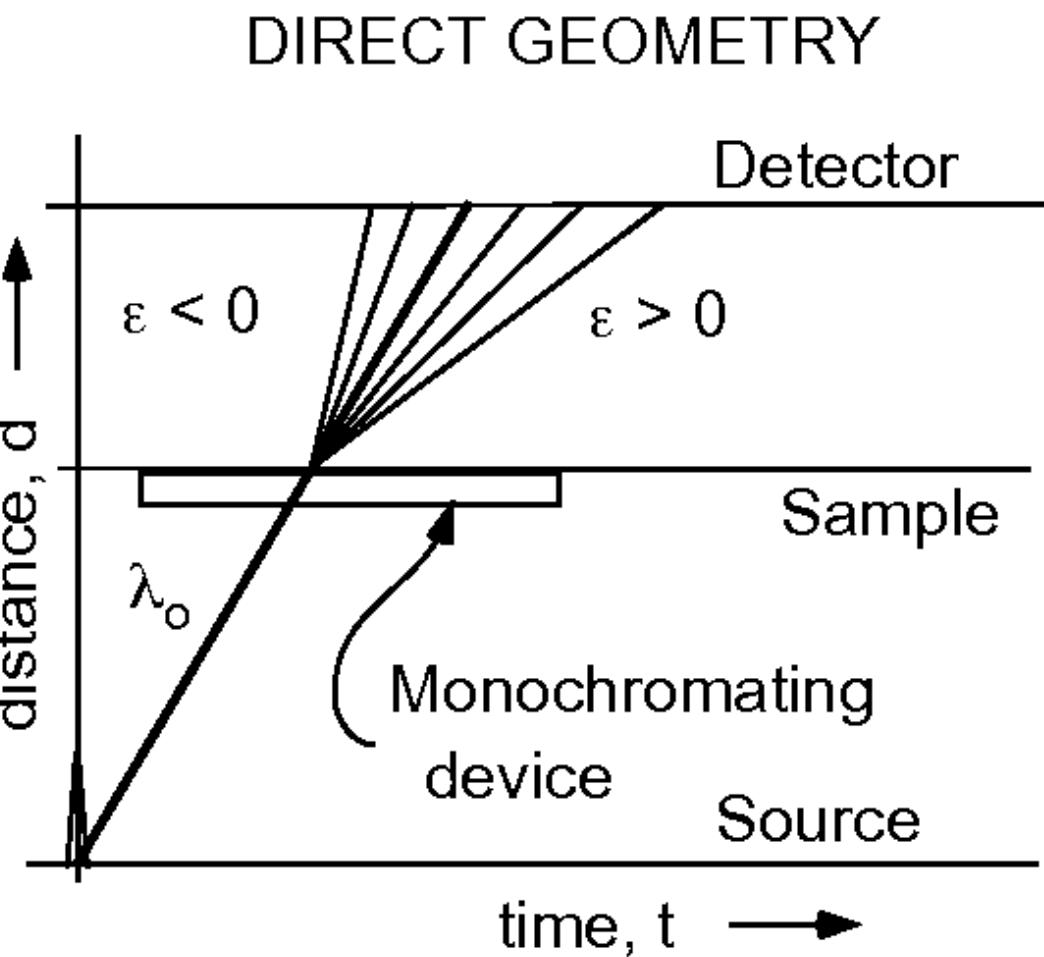
$$S(q, \omega) = \frac{d^2\sigma}{d\Omega dE}$$

Used to study dynamics



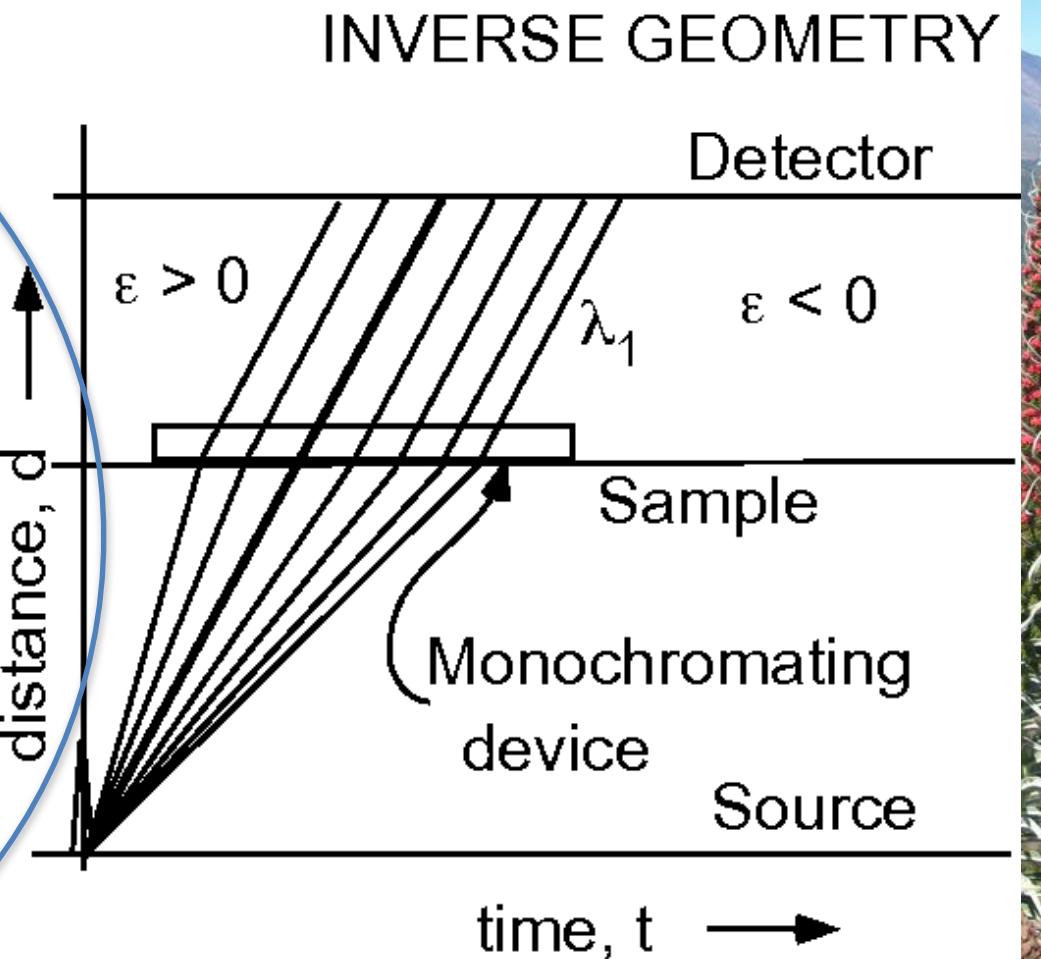
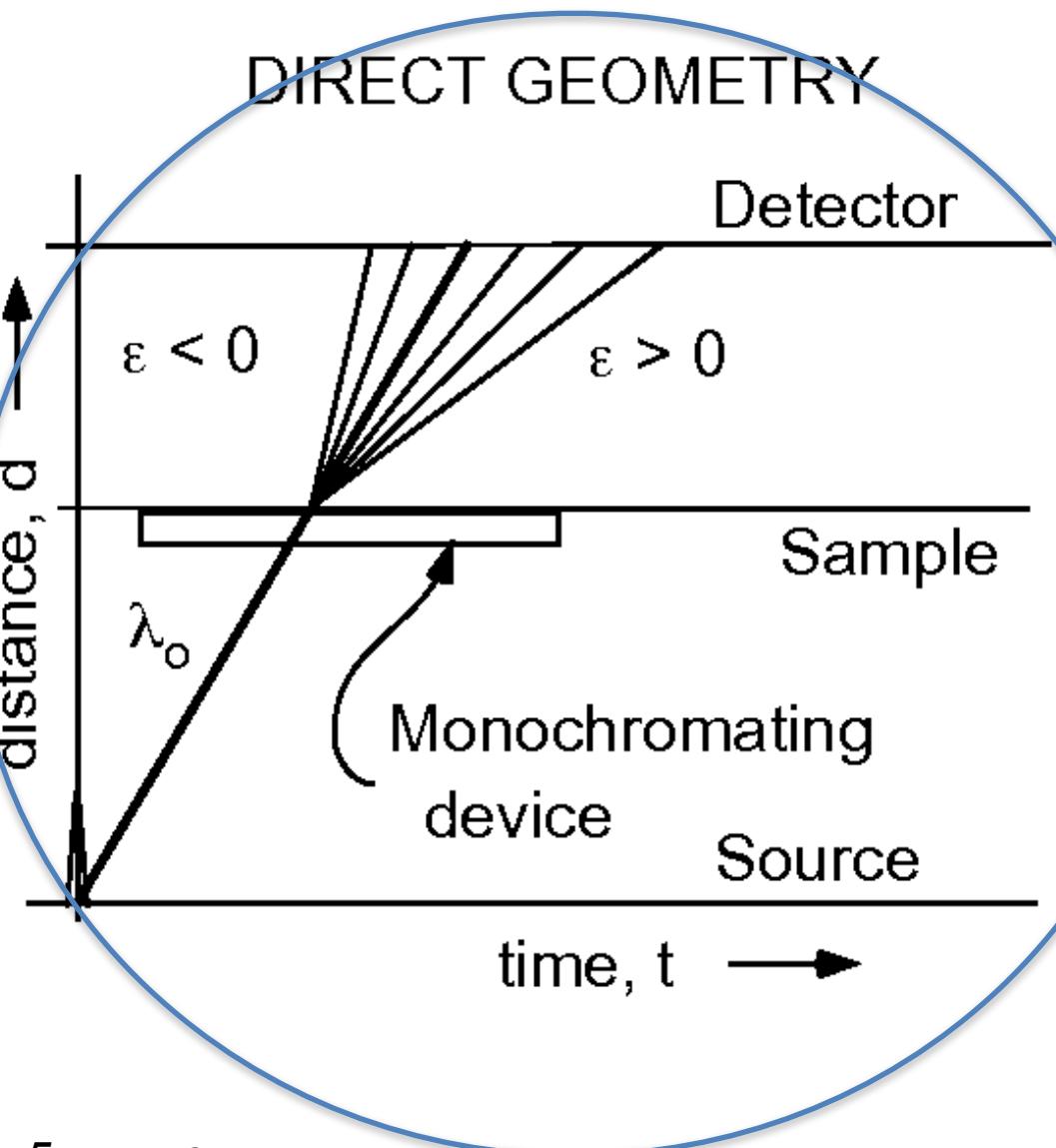


Direct vs. Indirect



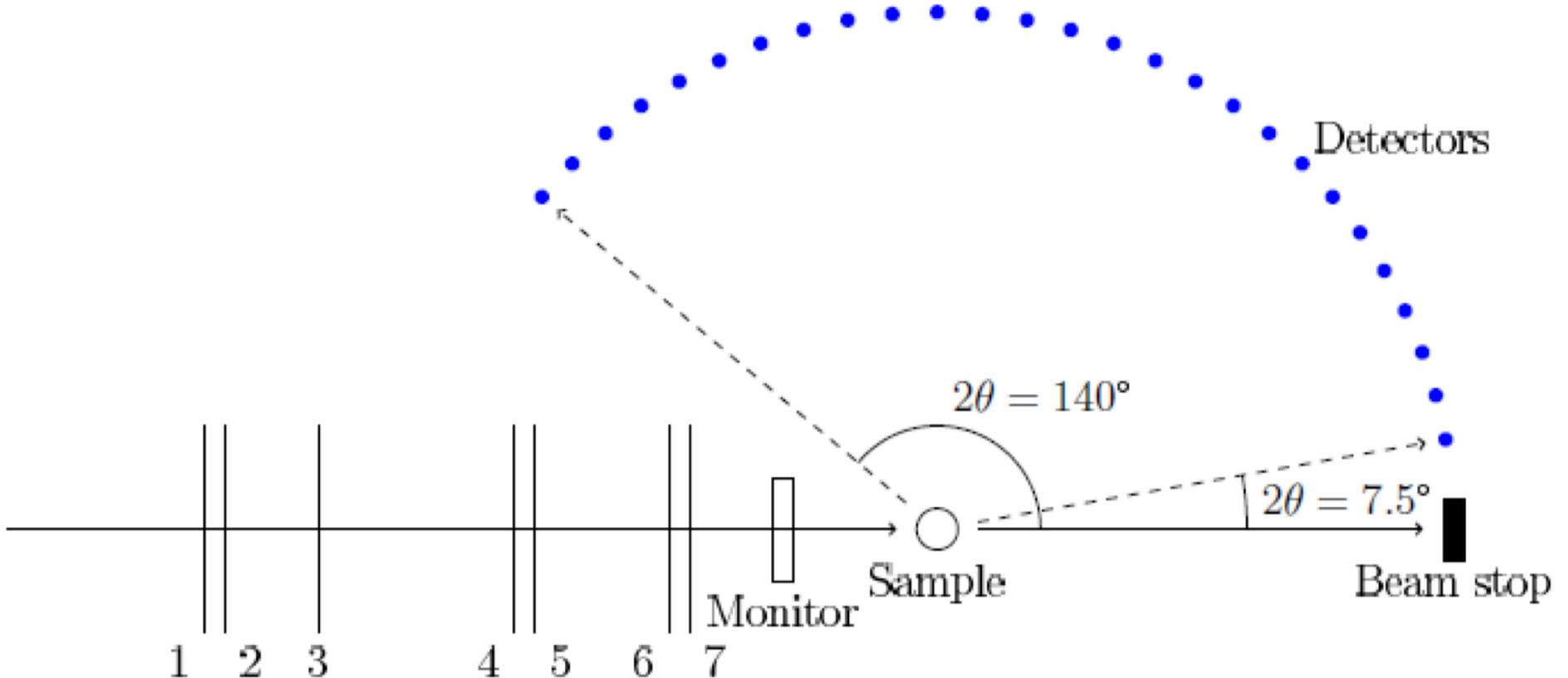


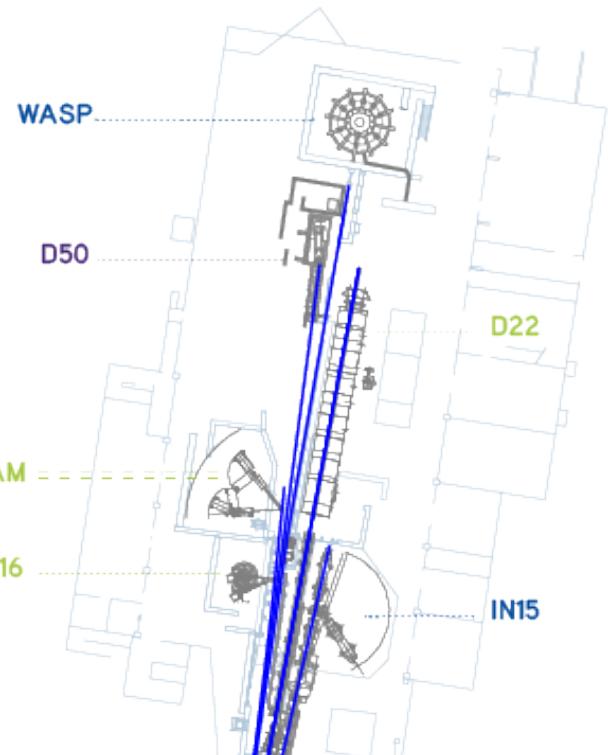
Direct vs. Indirect





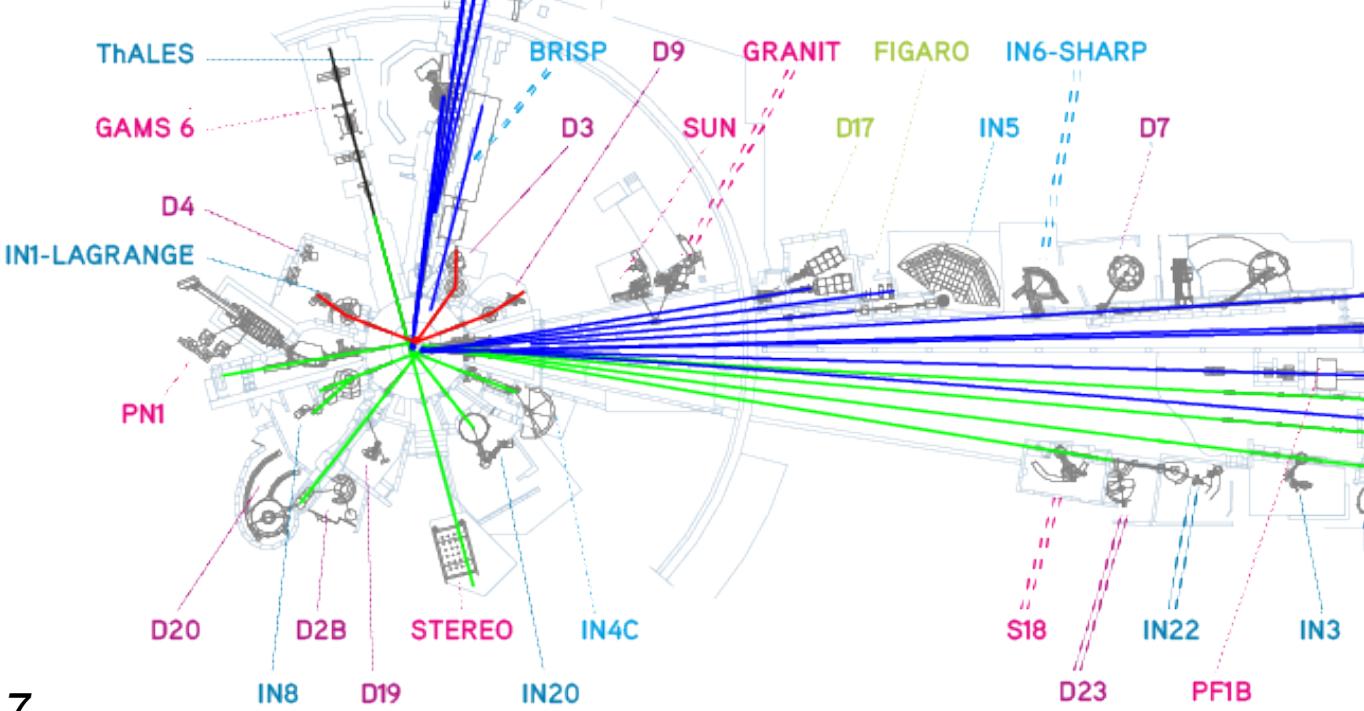
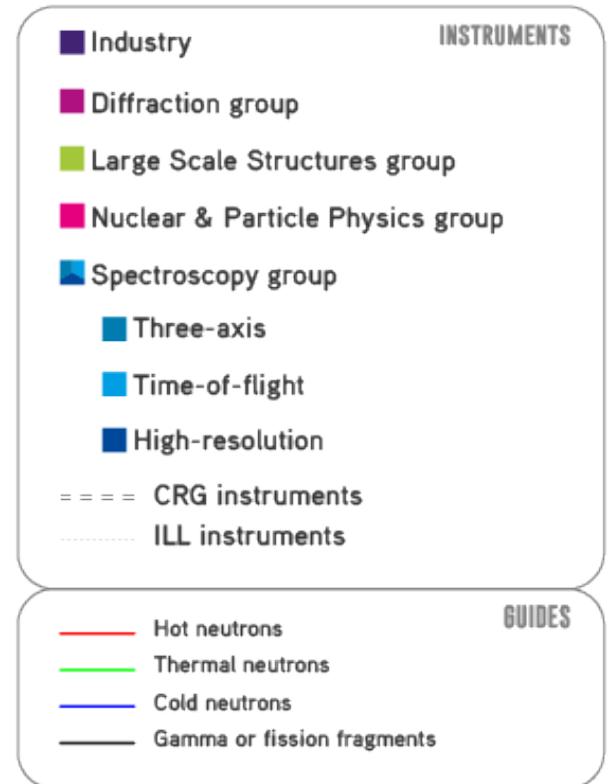
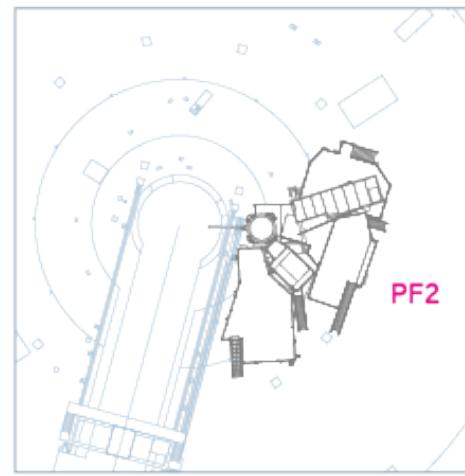
Direct geometry schematic

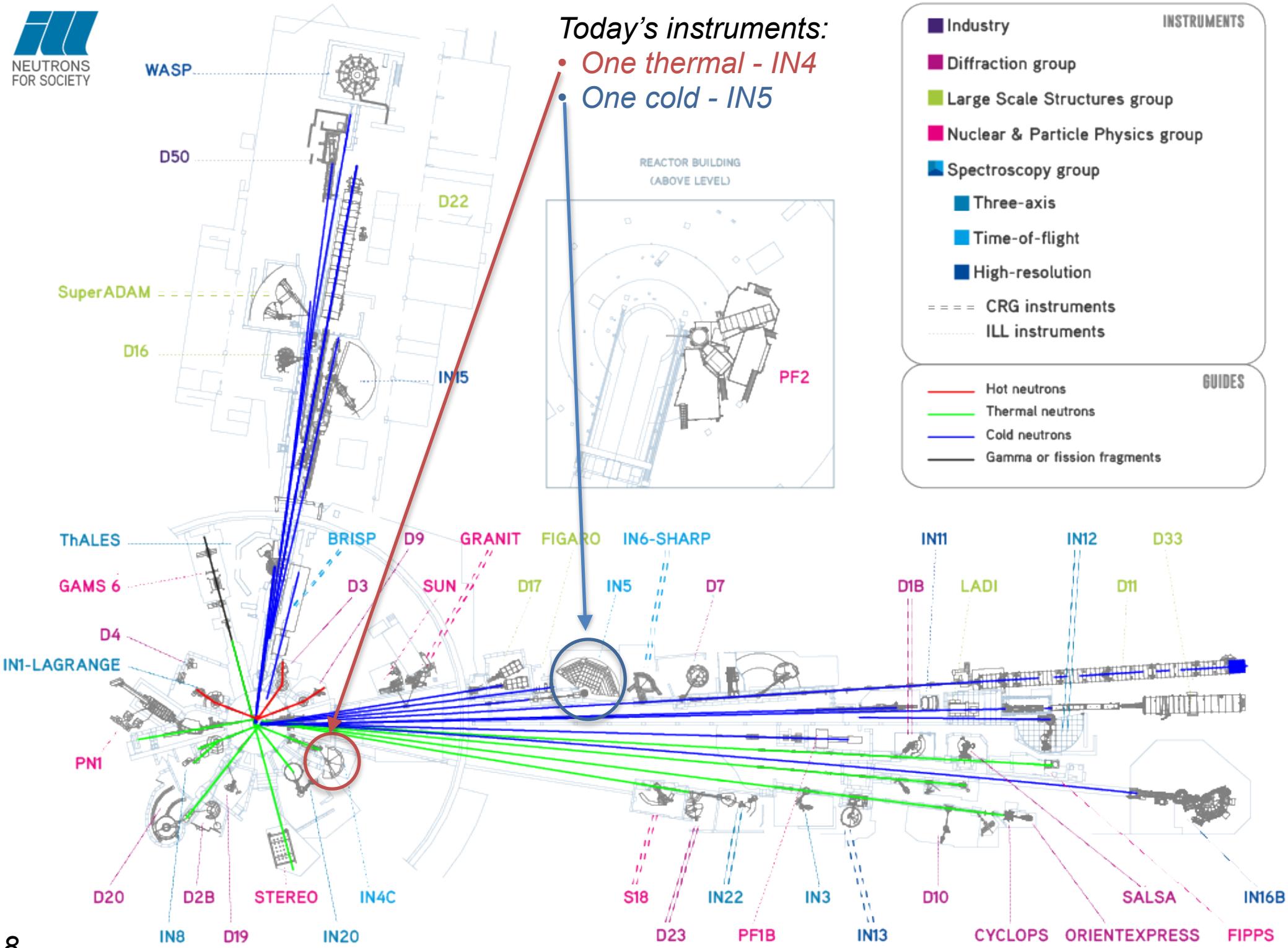




Today's instruments:

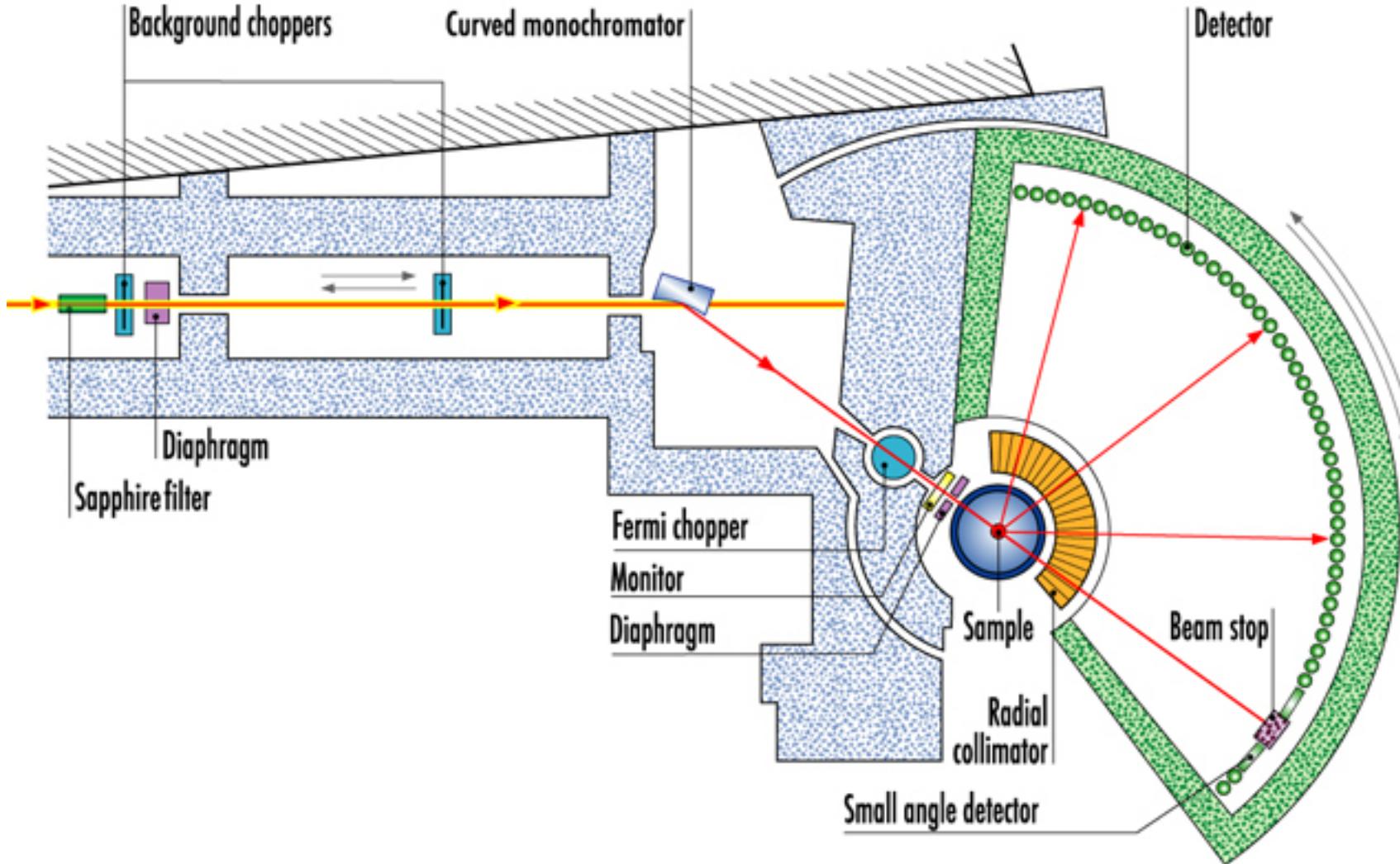
- One thermal
- One cold



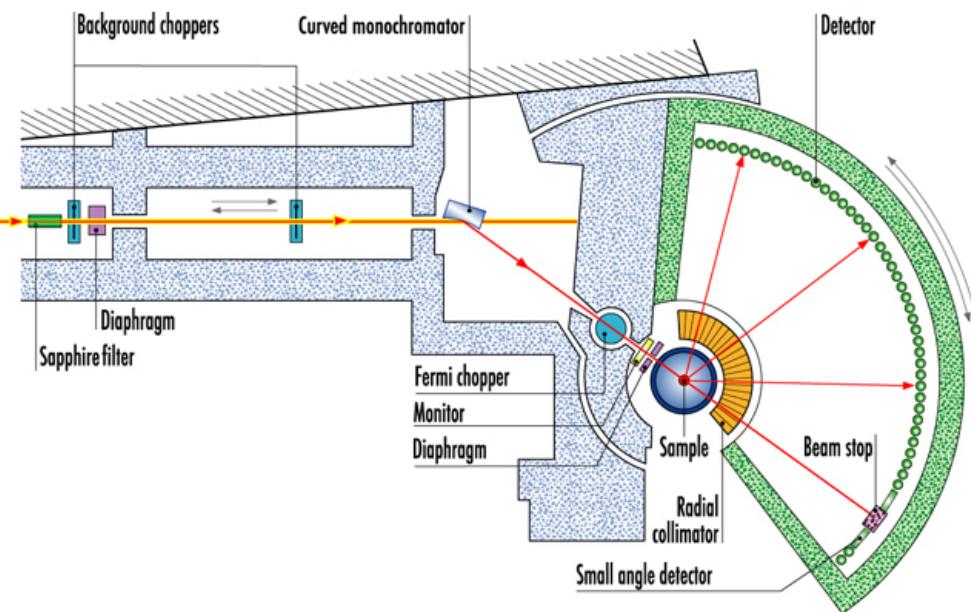




ILL IN4



ILL IN4



- Thermal, in ILL level C @ reactor face
- Use of chopper, focusing monochromator and fermi-chopper

IN4C - HIGH-FLUX TIME-OF-FLIGHT SPECTROMETER

IN4C is a high-flux time-of-flight spectrometer used for the study of excitations in condensed matter. It works in the thermal neutron energy range (10-100 meV).

Applications

- characterisation of interaction energies associated with bonding of atoms in solids and liquids;
- measurement of the energy level spacing in magnetic ions and of interaction between them;
- observation of the interaction of magnetic moments with their surrounding ions (crystal fields) or with conduction electrons (fluctuating valence, heavy fermions);
- determination of vibrational states in amorphous solids and polycrystals;
- examination of molecular excitations in various materials, also of technological interest (zeolites) and especially in diluted systems (matrix isolation).





McStas model

- | Get out 'Neutron Site -> ILL -> ILL_IN4.instr
- | Find the documentation for the instrument via Help -> mcdoc Component Reference
- | Run to compile, and visualise the instrument with mcdisplay-webgl
(Use setting in File->Preferences to set mcdisplay tool)
- | Look at the code in the editor





Special features

- In *DECLARE/INITIALIZE* there is infrastructure to generate an $S(q,\omega)$ with Dirac delta functions which is relevant for the current setting of the instrument
 - Accessible by running default parameters, specifically (sample_coh=Dirac2D.sqw. - the default)
- Run a simulation with default parameters and 1e7 neutron rays and inspect the output. Locate the detector output that illustrates the instrument resolution





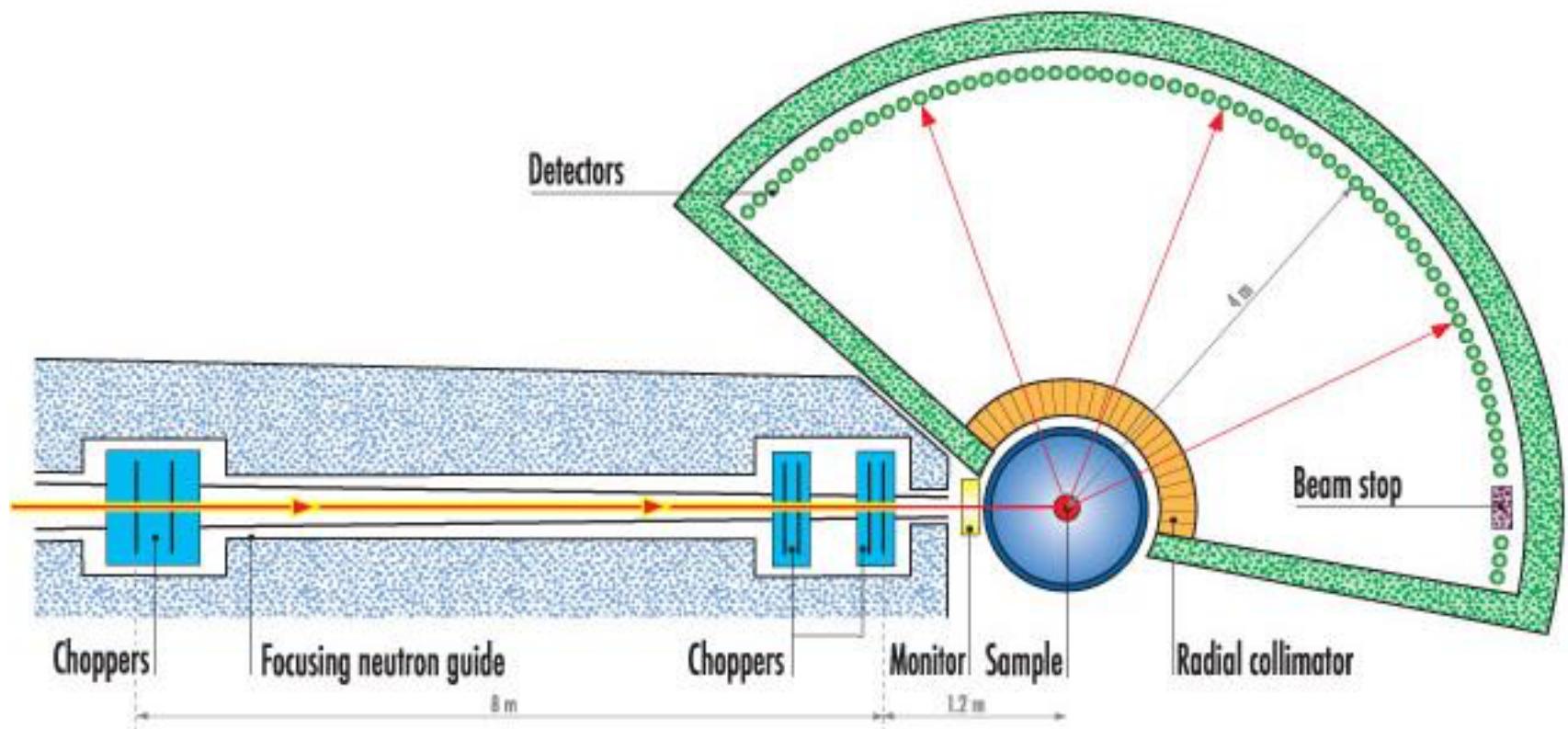
Investigate resolution @ different instrument settings

- | *Run simulations at $\lambda=1.1, 2.2, 3.3$ and 4.4 \AA*
- | *Hint:*
 - | *Look at instrument output and documentation, you may have to adjust e.g. monochromator type for non-default wavelength*
- | *Comment on the found differences*
- | *Optionally play with monochromator mosaicity*



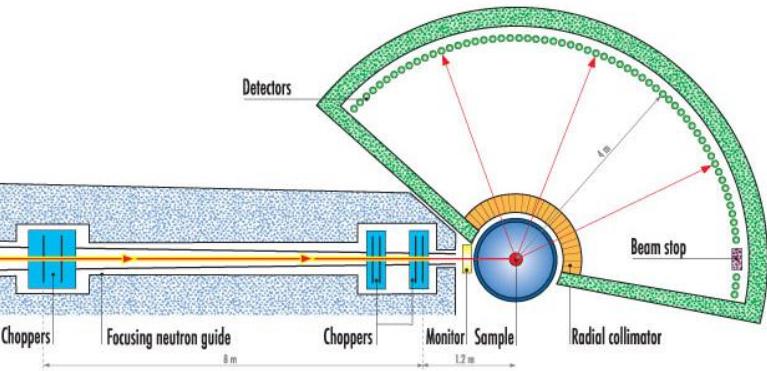


ILL IN5



ILL IN5

- Cold, in ILL7 guide hall
- On a guide with a 6-diskchopper setup



DISK CHOPPER TIME-OF-FLIGHT SPECTROMETER

IN5B is a high precision direct geometry Time-of-flight (ToF) spectrometer. It is used to study low-energy transfer processes as a function of momentum transfer.

Typically this instrument is used for measurements in the small energy and momentum transfer region with values of about 1 % for the energy resolution (e.g. quasi-elastic scattering in solids, liquids, molecular crystals and inelastic scattering with small energy transfers in the range 10 μ eV - 100 meV).

Applications

- Local and long-range diffusion in disordered systems such as liquids, molecular crystals, amorphous solids (superionic glasses, orientational glasses, spin glasses), polymers, hydrogen-metal systems, ionic conductors
- Dynamics of 'soft matter', including gels, proteins and biological membranes
- Dynamics of quantum liquids
- Rotational tunnelling in molecular crystals
- Crystal field splitting
- Spin dynamics in high-TC superconductors
- Critical scattering phenomena in dense gases and solids



ILL IN5 resolution

- | *Locate the ILL_IN5_Spots.instr in the Dropbox*
- | *Run the instrument as is, observing diffraction from powder lines*
- | *Also visualise the instrument using mcdisplay*





Enclosed modifications wrt. IN5 in McStas

- | Resolution mode ala IN4 simulation, accessible by input parameter RESO=1
- | Single-peak inelastic Dirac peak accessible by input parameters:
 - | ttspot (where to point the peak in angle)
 - | nspots (how many spots to define)
 - | wspot (magnitude of energy exchange)



Perform studies of resolution, IN5



- Use your gathered experience from the earlier IN4 simulations
- Comment on the qualitative difference to the resolution function from IN4





Investigate resolution properties via Spot_sample

- Run a simulation with
 - $nspots=1$ (one discrete inelastic spot)
 - $wspot=1$ (energy-transfer 1meV)
 - $ttspot=-60,60$ (vary spot position qvalue)
 - $-N13$ (13 scan steps)
- Investigate influence of sample size (reduce height and radius parameters)





Investigate resolution properties via Spot_sample

- *Inelastic: Run a simulation with*
 - *nspots=1 (one discrete inelastic spot)*
 - *wspot=1,4 (energy-transfer 1meV to 4meV)*
 - *ttspot=0 (vary spot position qvalue)*
 - *-N21 (21 scan steps)*
- *Optionally launch iFit/Matlab and load data from one or more of the TOF monitor outputs of the scan, e.g.*
 - *a=iData('folder/5/in5*.t')*
 - *a.error=1*
 - *fits(a,'gauss')*
 - *plot(a)*





Access to McStas TOF Spectras and more in Mantid

- | *Simple recipe to generate Mantid-compatible NeXus files for Mantid available at*
<https://github.com/McStasMcXtrace/McCode/wiki/McStas-and-Mantid>
- | *Includes both your normal McStas monitors as histogram but also handles event-data*
- | *Examples already in McStas:*
 - | *SNS_ARCS.instr (with Spot_sample)*
 - | *ILL_IN5_Mantid.instr*
 - | *templateSANS_Mantid.instr*





Optional exercises - 1

| Use *ILL_IN5_Mantid* to generate *Mantid* output via:

1. Define compilation with NeXus support

```
export MCSTAS_CFLAGS="-g -fPIC -O2 -DUSE_NEXUS -I$NEXUS"
```

2. Compile your instrument

```
mcrun.pl -c ILL_IN5_Mantid.instr -n0
```

3. Generate an IDF file for use with Mantid

```
mcdisplay.pl ILL_IN5_Mantid.instr --format=Mantid -n0
```

4. Run your simulation with NeXus output

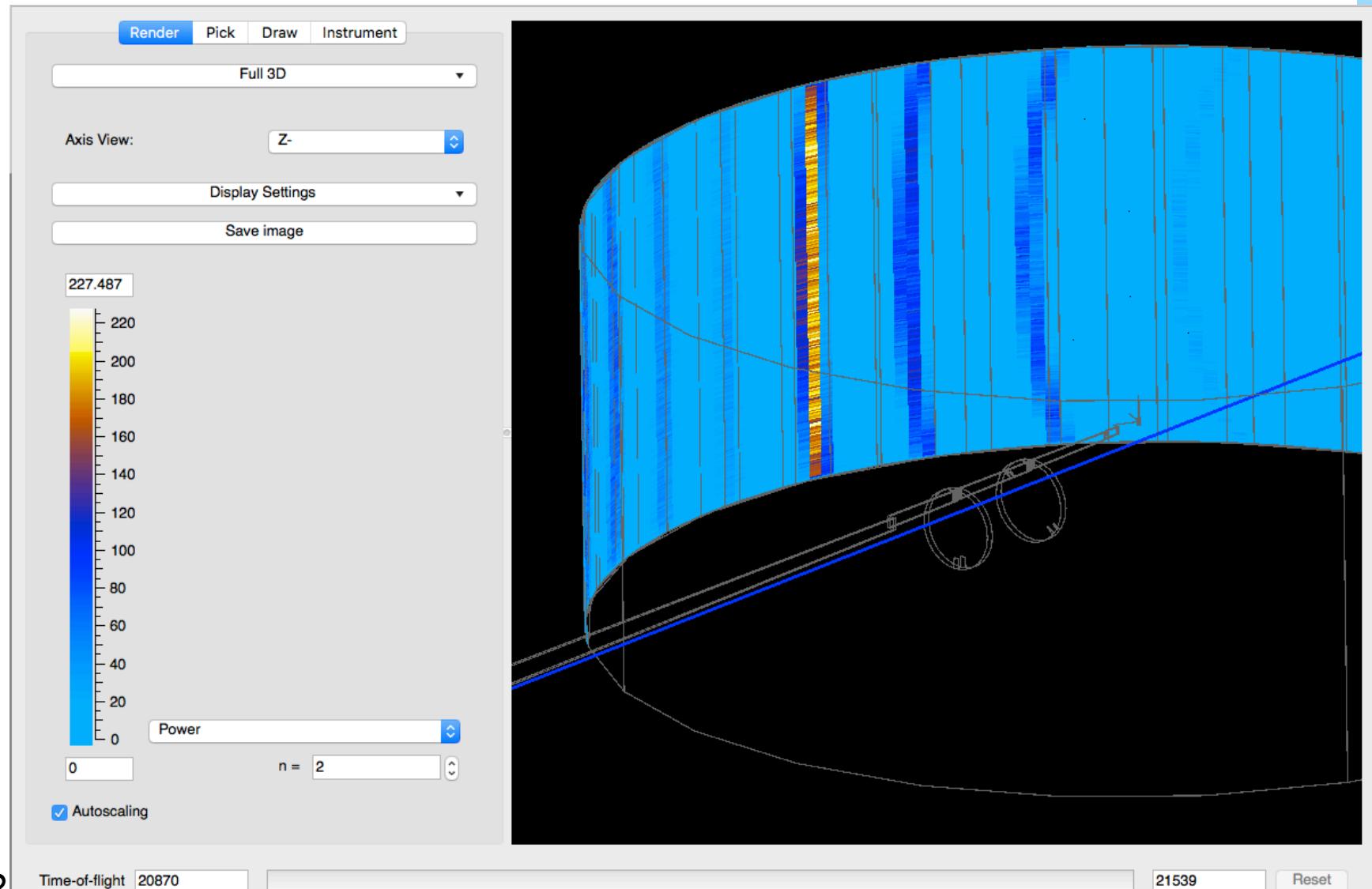
```
mcrun.pl ILL_IN5_Mantid.instr -n1e7 --format=NeXus
```





Optional exercises - 1

Handle your output in Mantid



Optional exercises - 2



- | Use the recipe from
- | <https://github.com/McStasMcXtrace/McCode/wiki/McStas-and-Mantid>
- | to enable Mantid-output in *ILL_IN4.instr*

