Erik Knudsen

TOF spectrometer (direct geometry)

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Spectroscopy reminder

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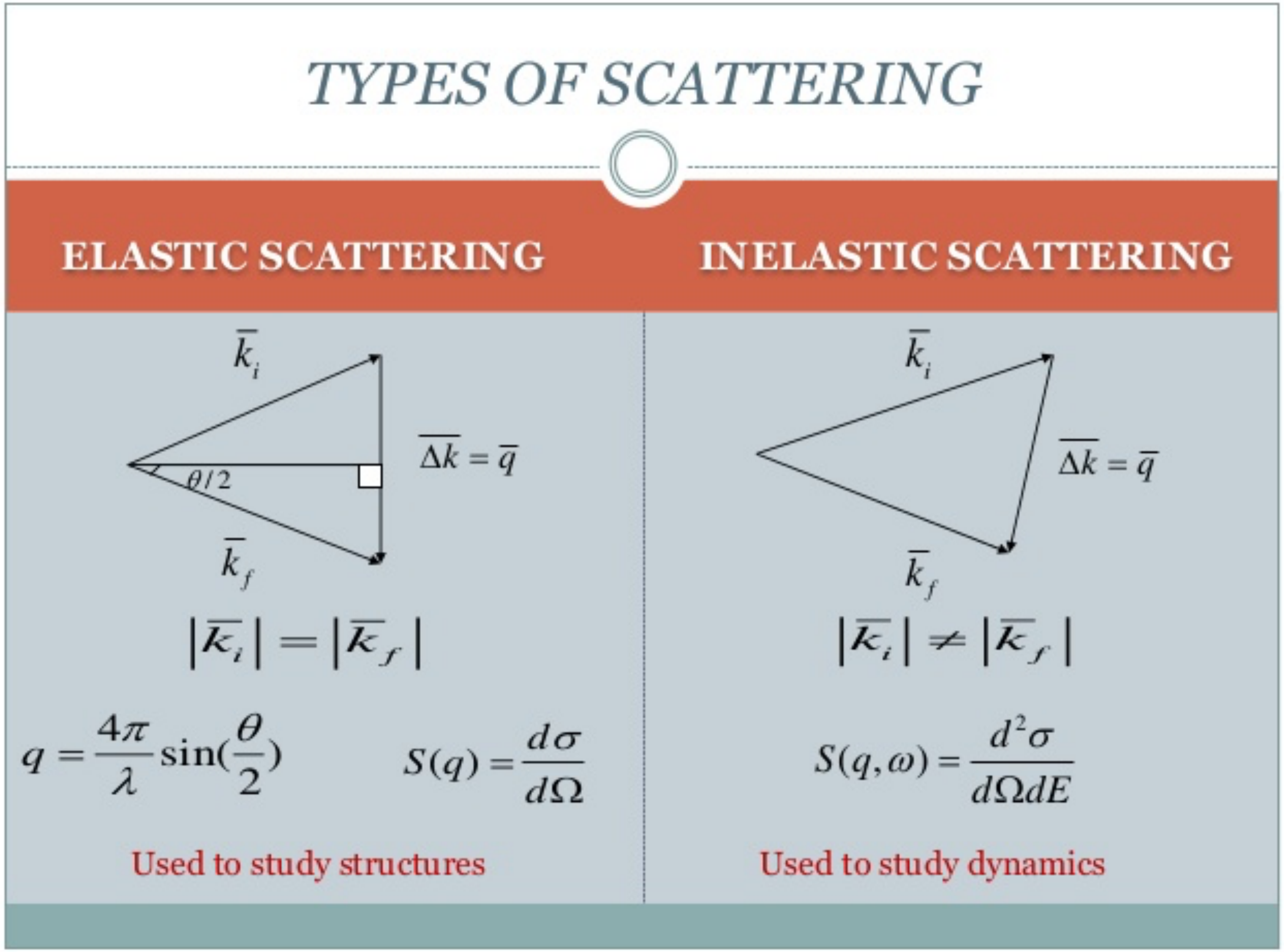
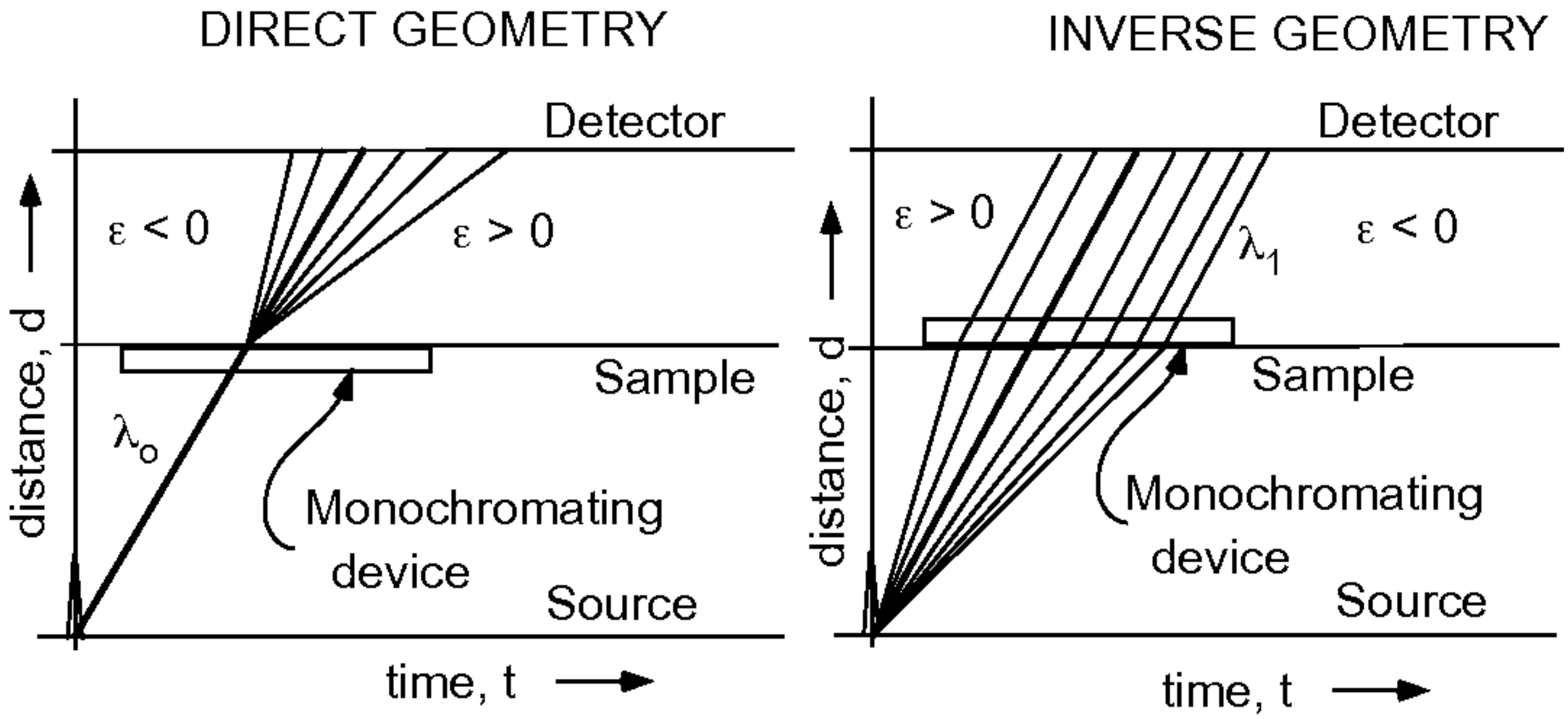


Direct vs. Indirect



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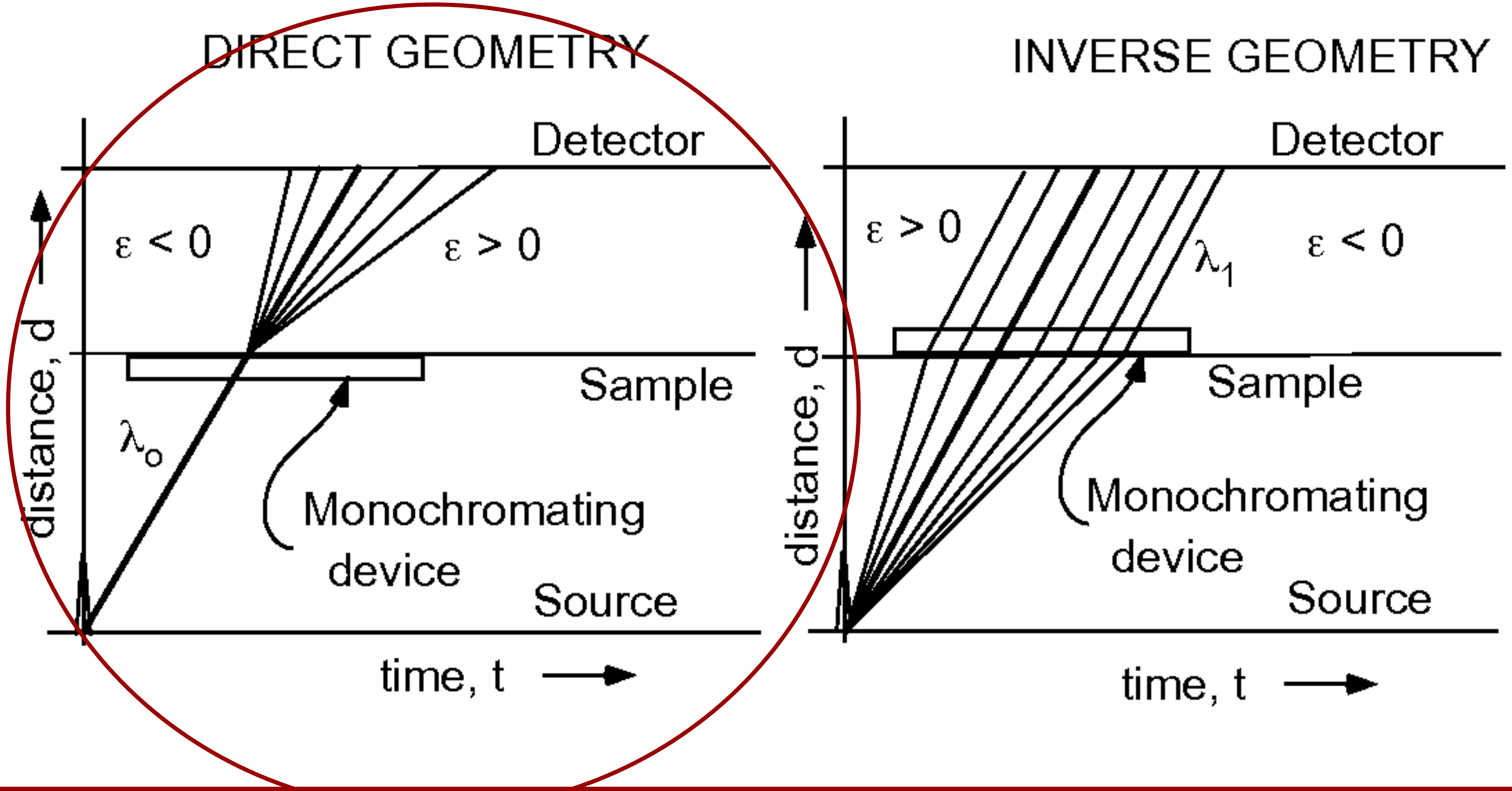
Direct vs. Indirect



Useful links / docs

- http://mcstas.org/links

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- Tutorial: Build a diffractometer (outdated in certain parts)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**

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Variant	Type	2D/3D	Special cmdline switches	ToF mode
mcdisplay- pyqtgraph	Python 3 + pyqtgraph	2D x 3 planes	`--invcanvas` (invert colors)	`--tof` `--TOF` `--ToF`
mcdisplay.pl (mcplot-pl on Windows)	Perl 5 + PGPLOT	2D x 3 with PGPLOT, 3D with Matlab	`-pPLOTTER --format=PLOTTER` can be used to forward output to PGPLOT, Gnuplot, Matlab, ... `-ps/-psc/-gif` save hardcopy `--complete` When outputting XML, also describe component geometry `--tmax=VAL` ToF axis limit when in --TOF mode	`--TOF/-T`

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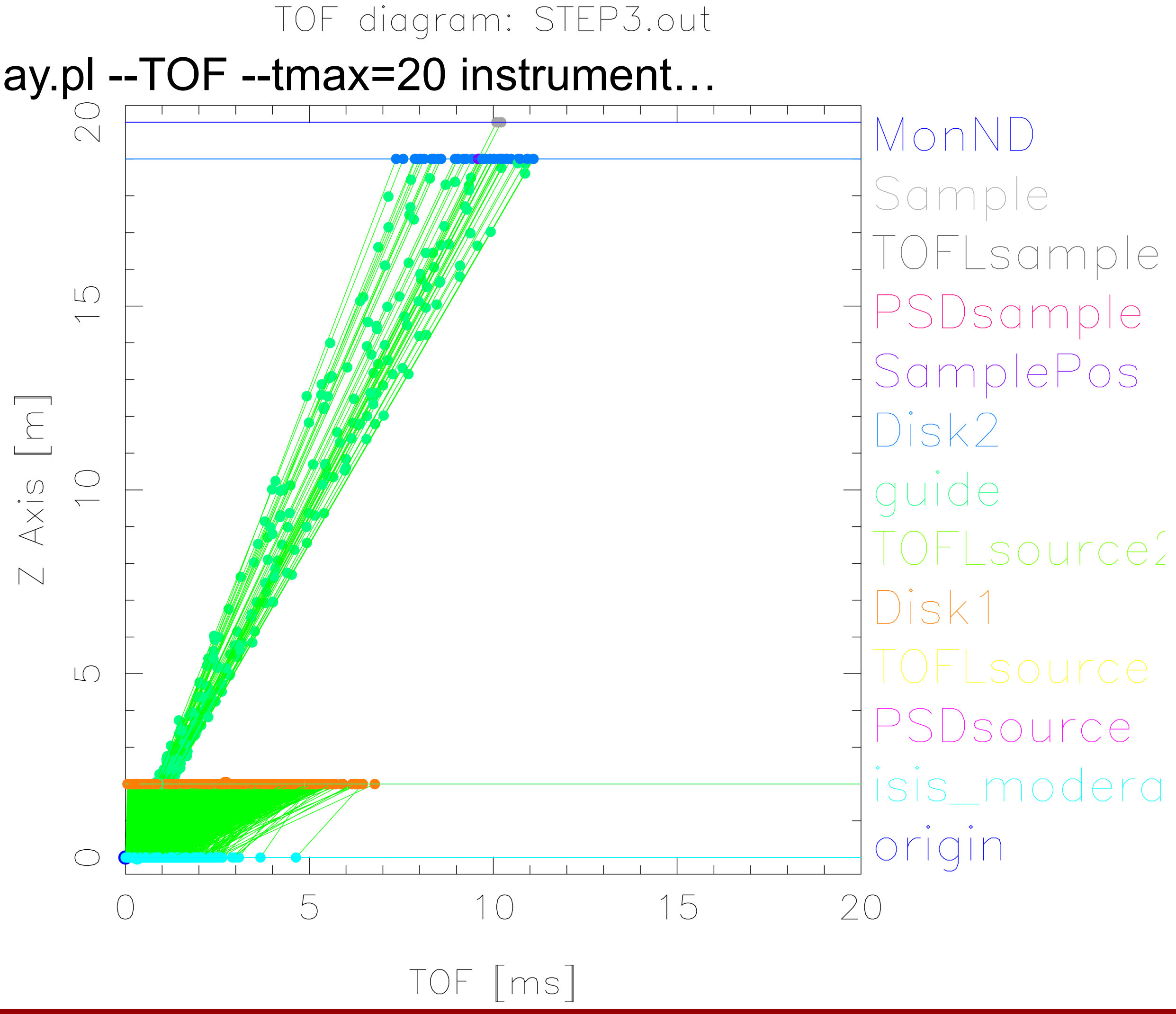
TOF diagram util based on mcdisplay

- mcdisplay.pl --TOF --tmax=20 instrument…



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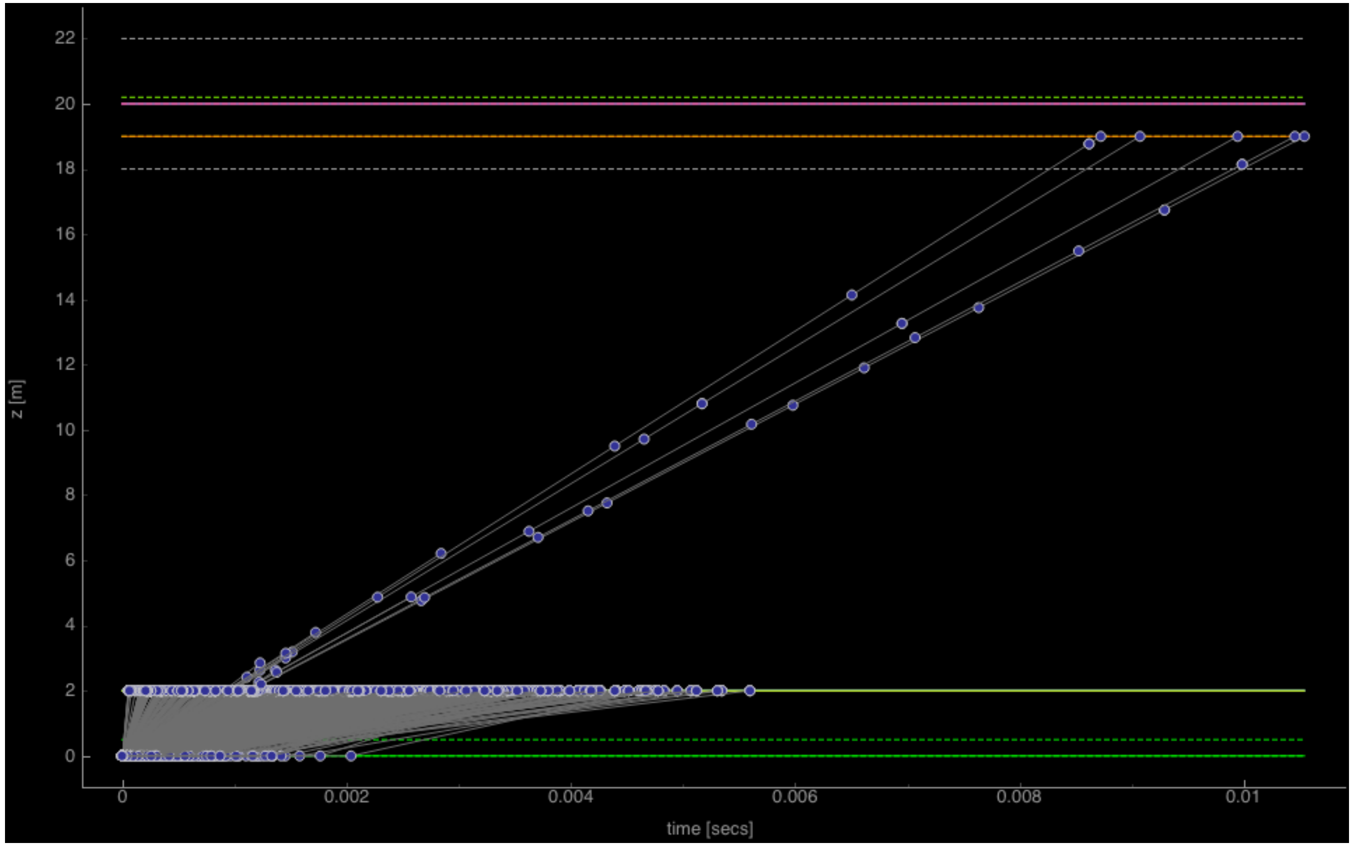
TOF diagram util based on mcdisplay

- mcdisplay-pyqtgraph --TOF instr



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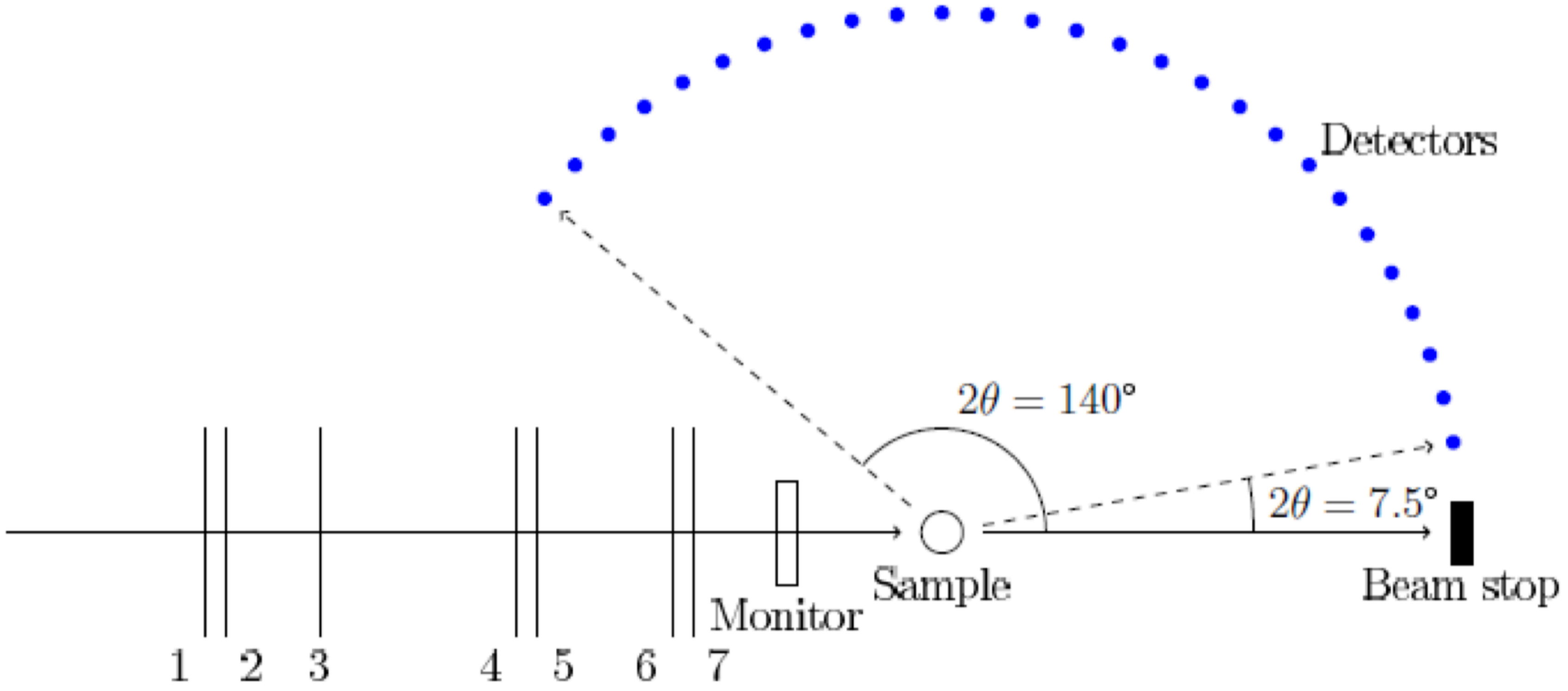
Direct geometry schematic



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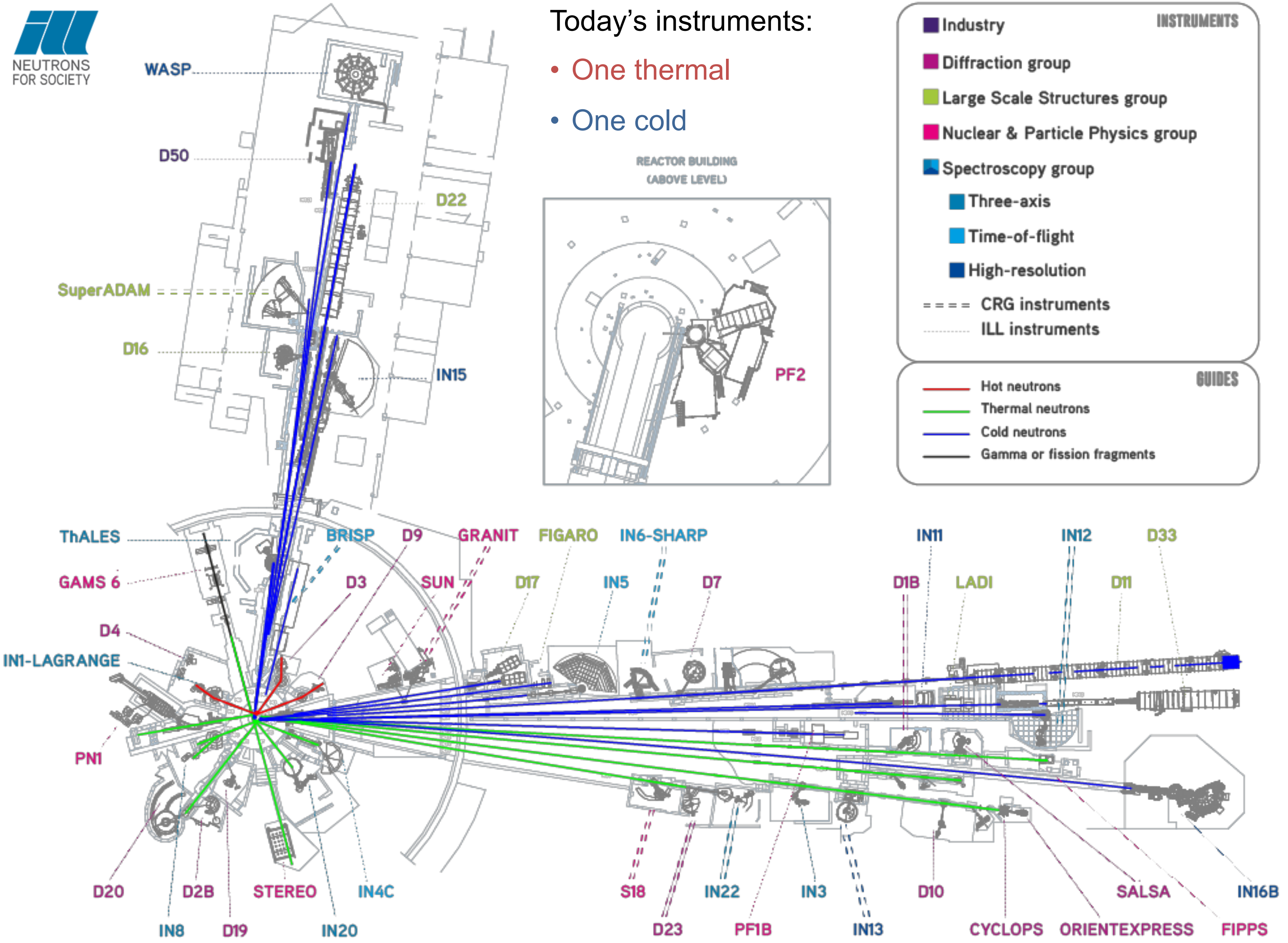
Today's instruments:

- One thermal
- One cold



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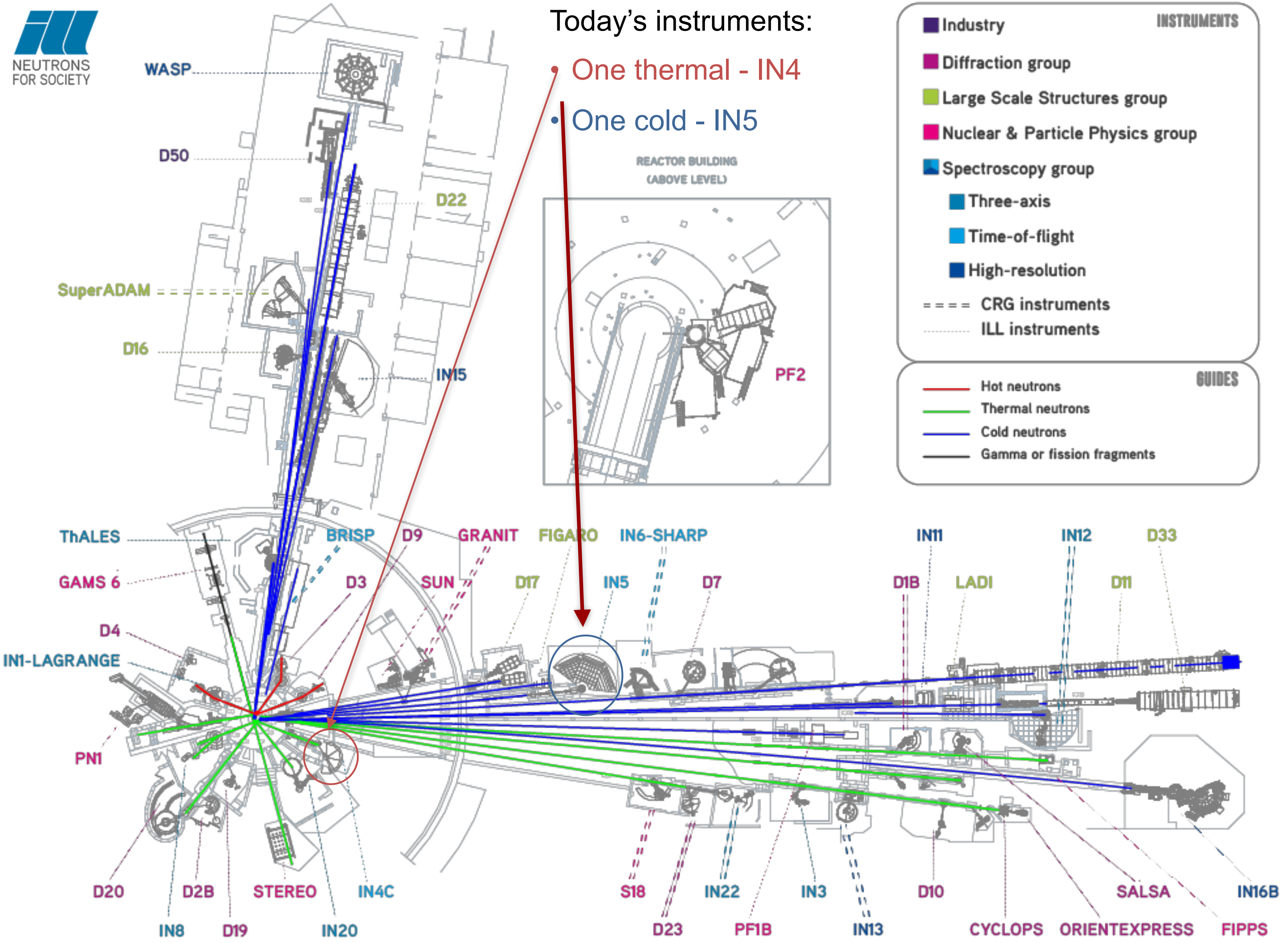
Today's instruments:

- One thermal - IN4
- One cold - IN5



EUROPEAN SPALLATION SOURCE

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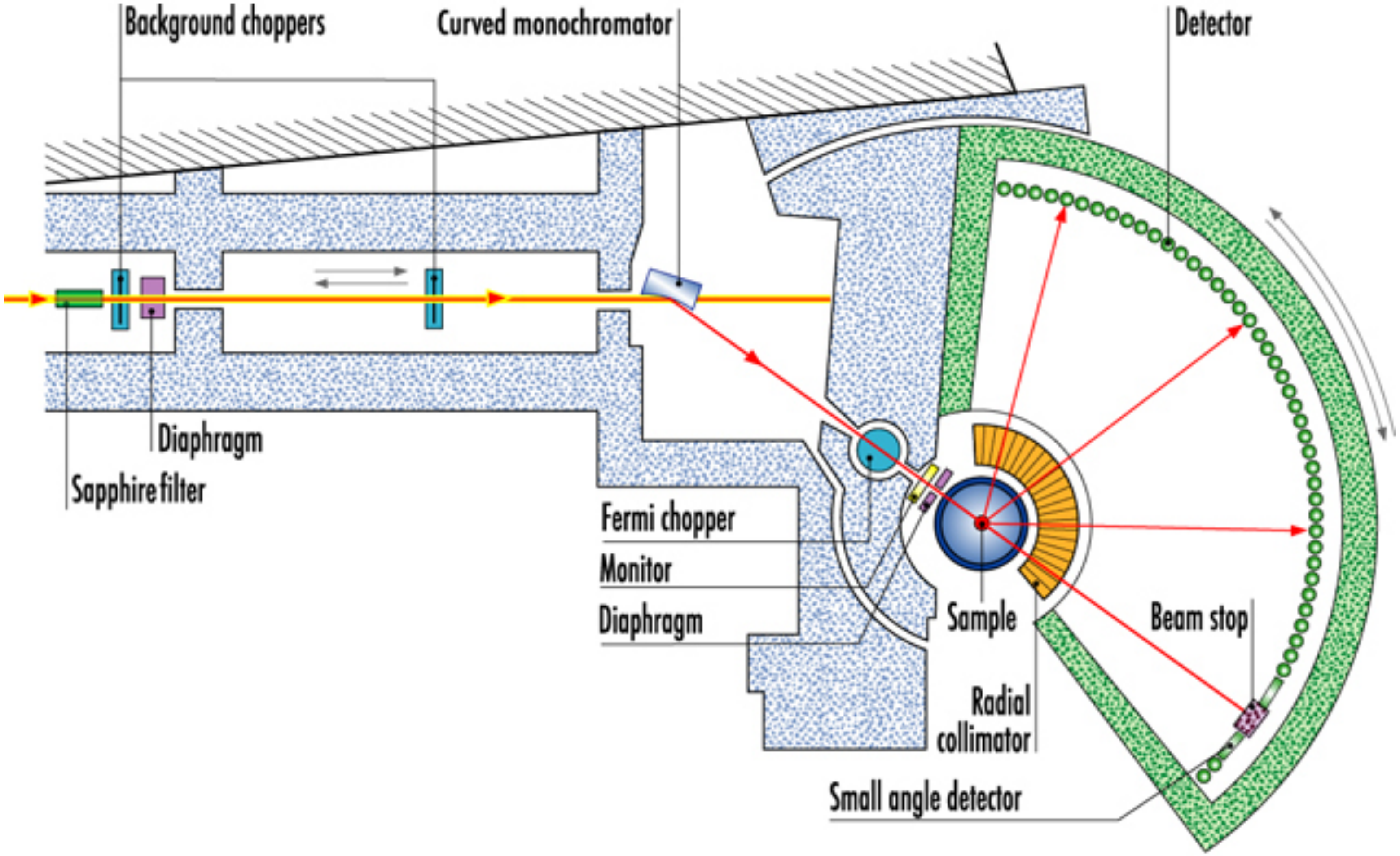
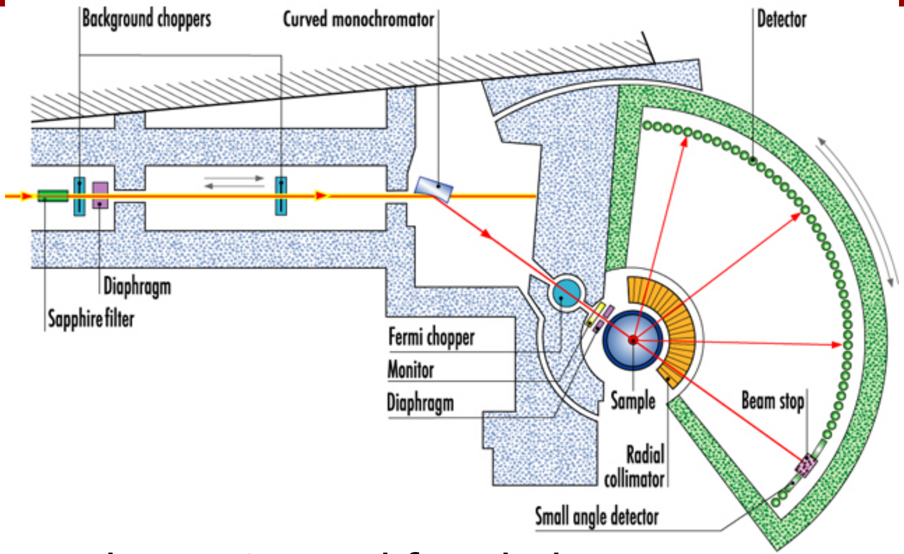


ILL IN4



- 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).

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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

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Special features

- In DECLARE/INITIALIZE there is infrastructure to generate an S(q,ω) 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

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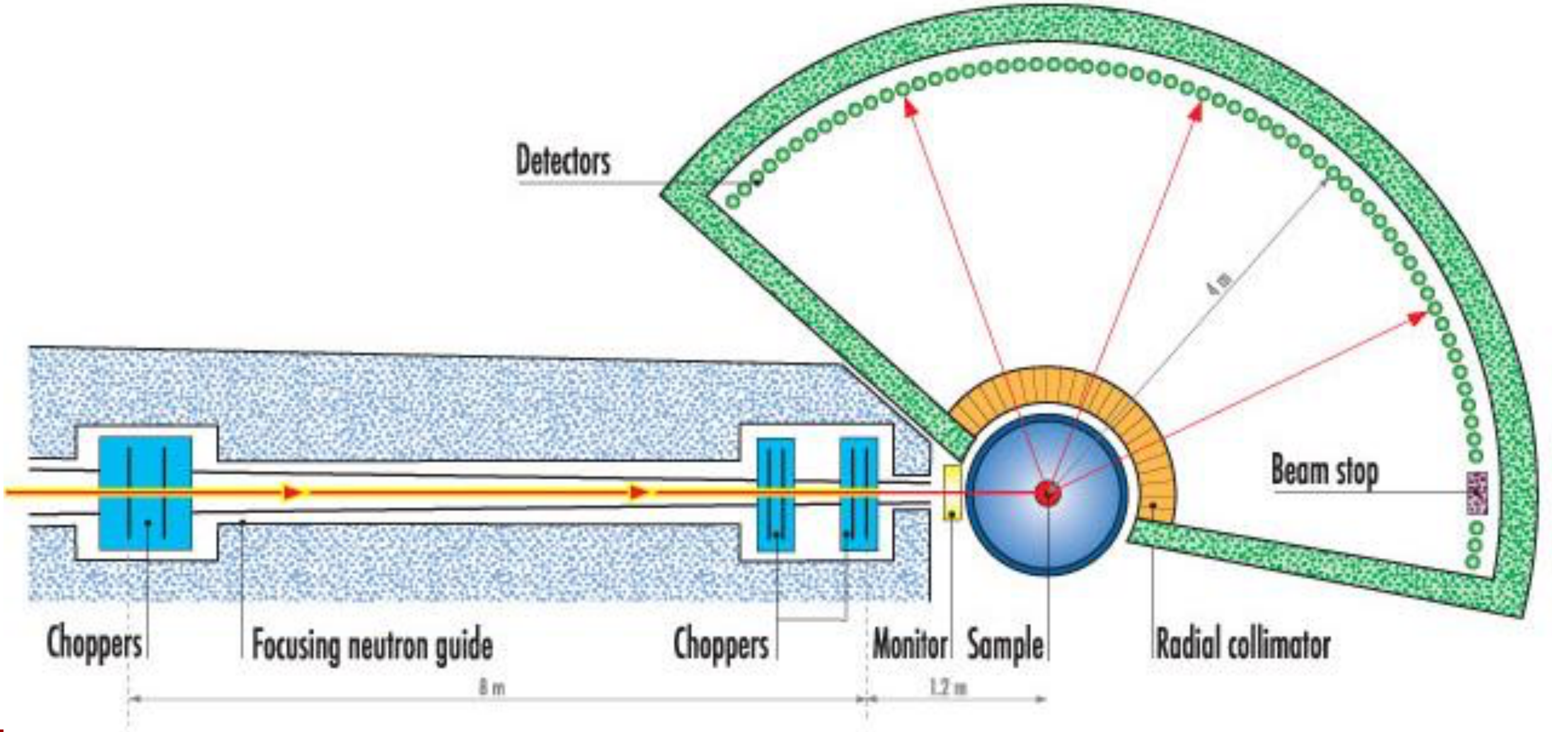
Investigate resolution @ different instrument settings

- Run simulations at lambda=1.1, 2.2, 3.3 and 4.4 Å
- 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



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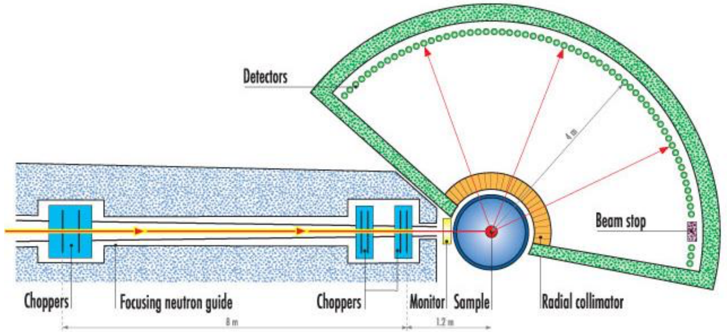
ILL IN5



- 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 µeV - 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

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ILL IN5 resolution

- Use the ILL_IN5_Spots.instr from your local McStas
- Run the instrument as is, observing diffraction from powder lines
- Also visualise the instrument using mcdisplay

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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

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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)

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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)

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