Optimisation of NR and SANS Instrumentation

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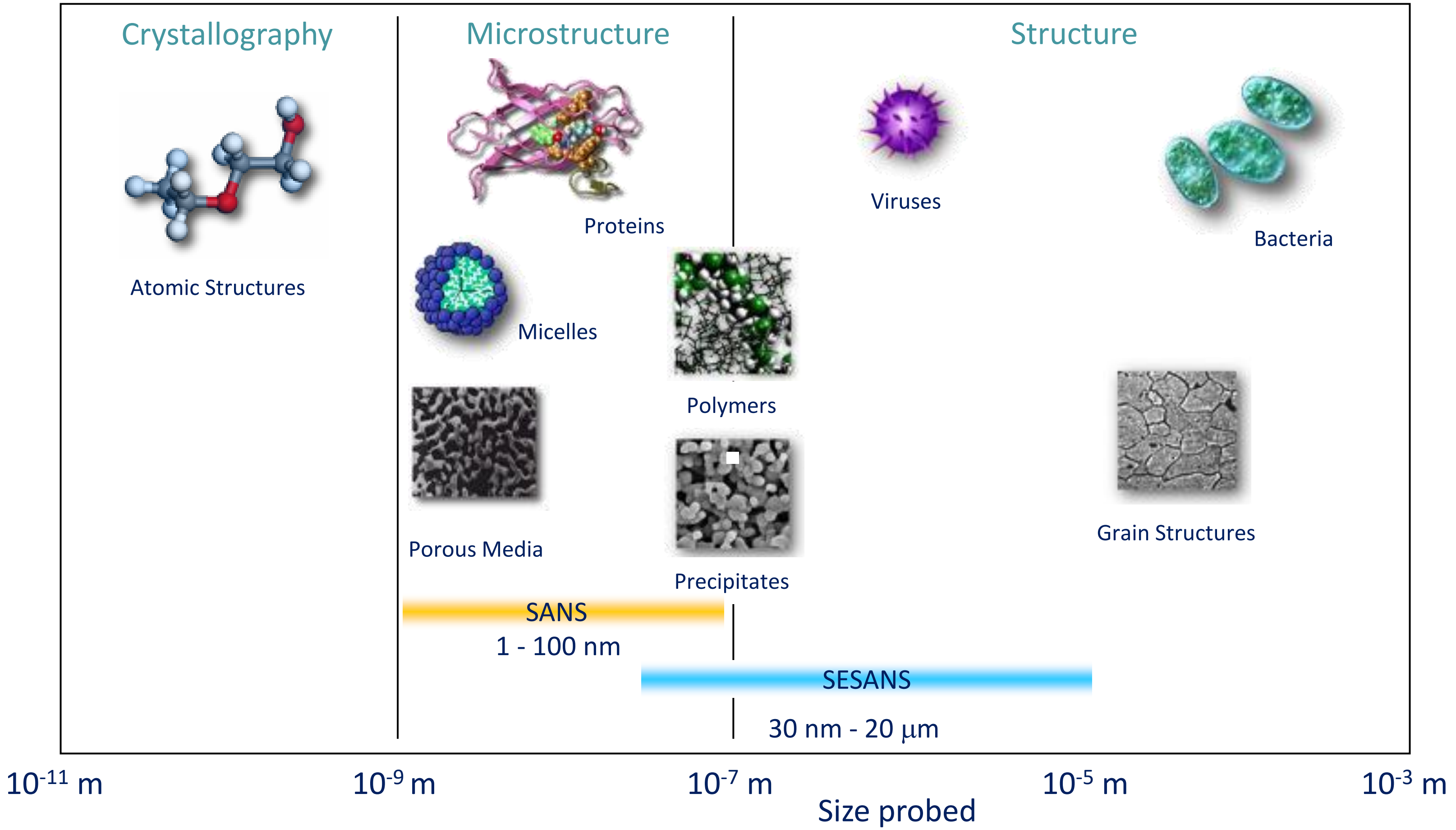
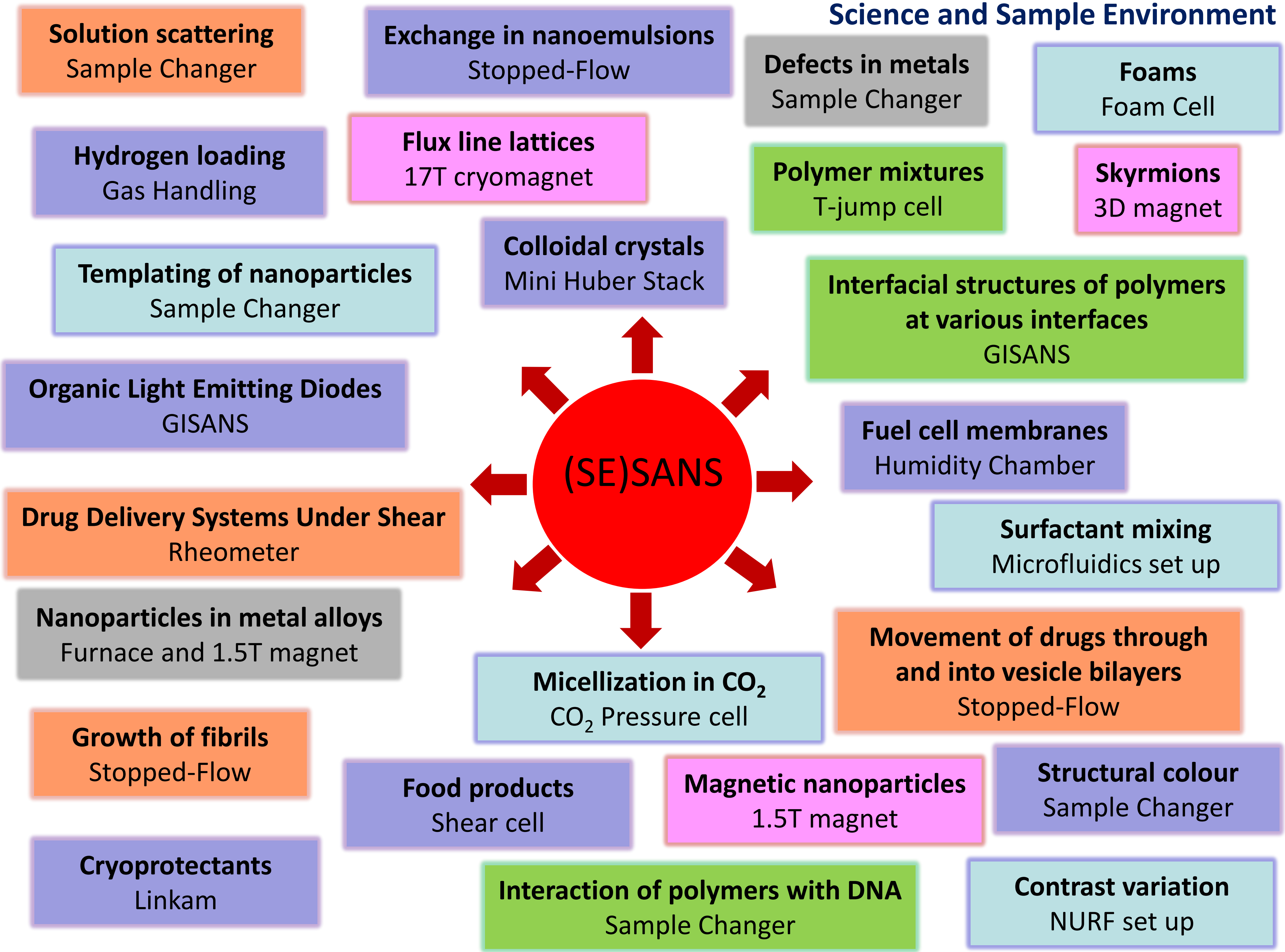
ISIS

SANS

- Length scales probed - 1s to 100s nm
  - Studies include surfactants, polymers, liquid crystals, nanoparticles, lipids and fibres.

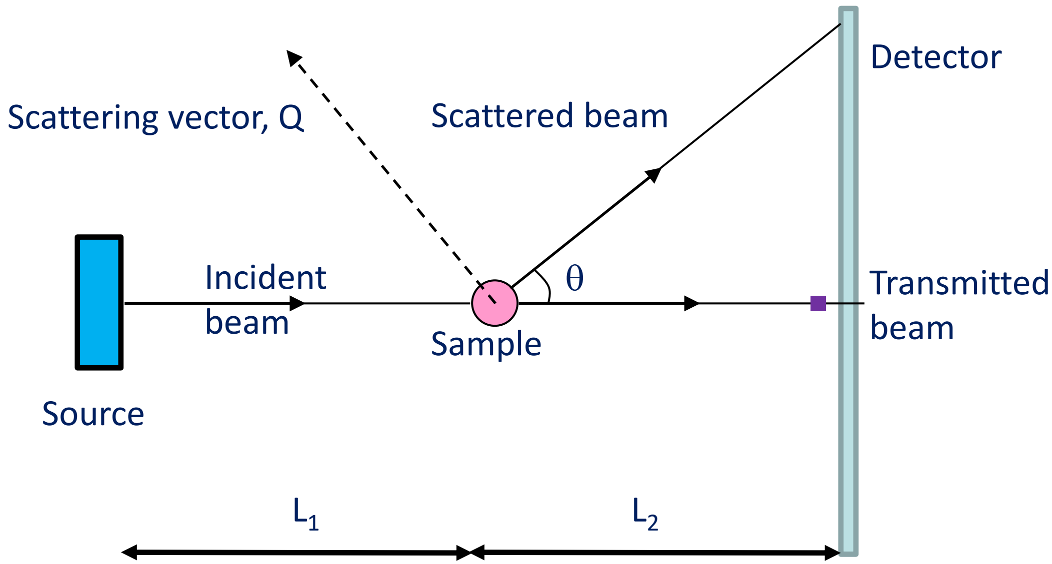


Science and Sample Environment



SANS In Transmission Geometry

- Lengthscales are explored in reciprocal space by detecting the number of scattered neutrons as a function of the scattering vector, *Q*.



Units are either $Å^{-1}$ or nm^{-1} i.e. the smaller the value of *Q* the bigger the object

Q is also related to wavelength and the scattering angle by:

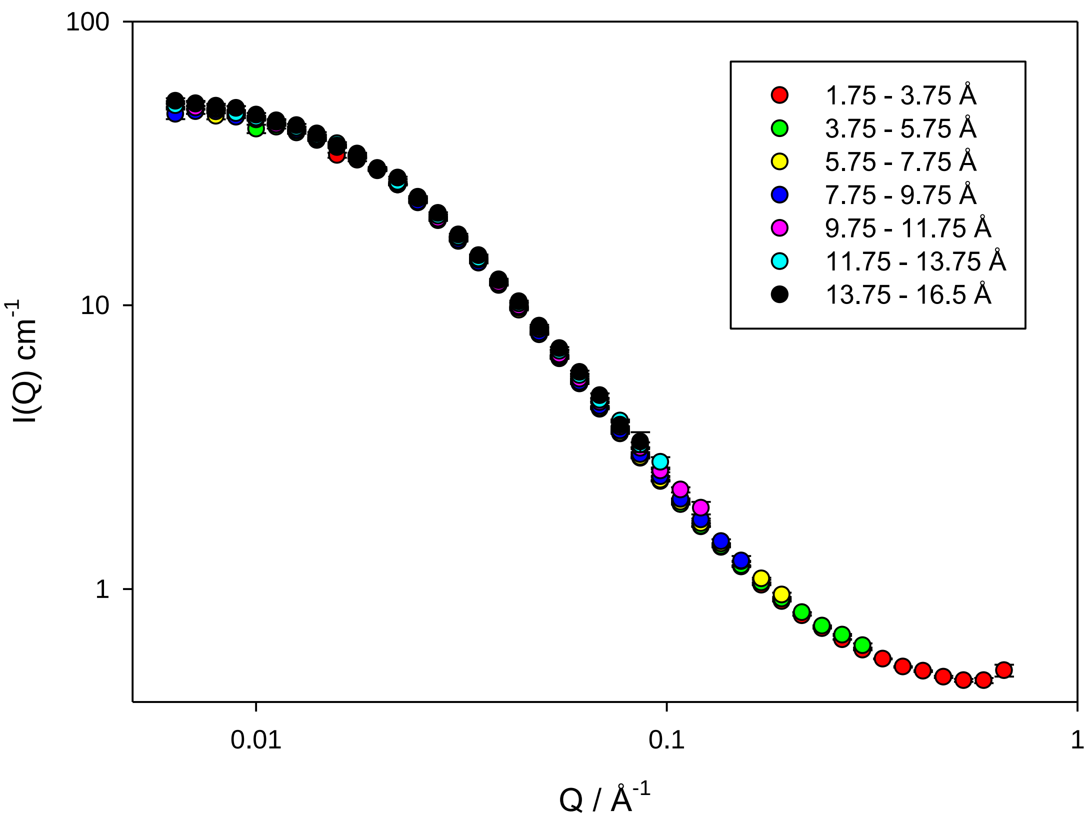
$$Q = \frac{4\pi \sin\left(\frac{\theta}{2}\right)}{\lambda}$$

Q (size) range is varied by altering θ or λ

- $L_1 = L_2$ for optimal *Q* resolution
- To reach the smallest *Q* values the incident flux is always lower in conventional ‘pinhole collimation’ SANS as a long incident collimation is needed

Time-of-Flight

- At ISIS we use time-of-flight (TOF) to record numerous diffraction patterns at different wavelengths, then we combine the patterns at different wavelengths onto a single Q scale
- TOF SANS therefore has a wide Q range in a single measurement



On Sans2d:

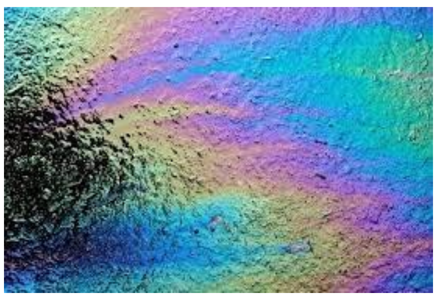
- Wavelength range = 1.75 – 16.5 Å
- 2 x 1m^2 detectors
- Q-range = 0.001 – 3 $Å^{-1}$ - dependent on detector positions

Need wavelength dependent corrections for:

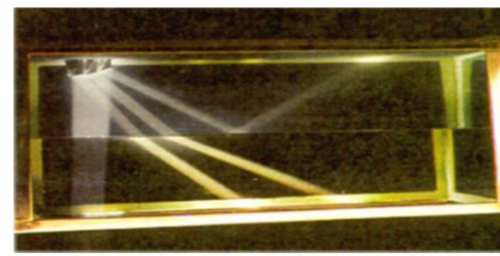
- Monitor spectrum
- Detector efficiency
- Sample transmission (measured)

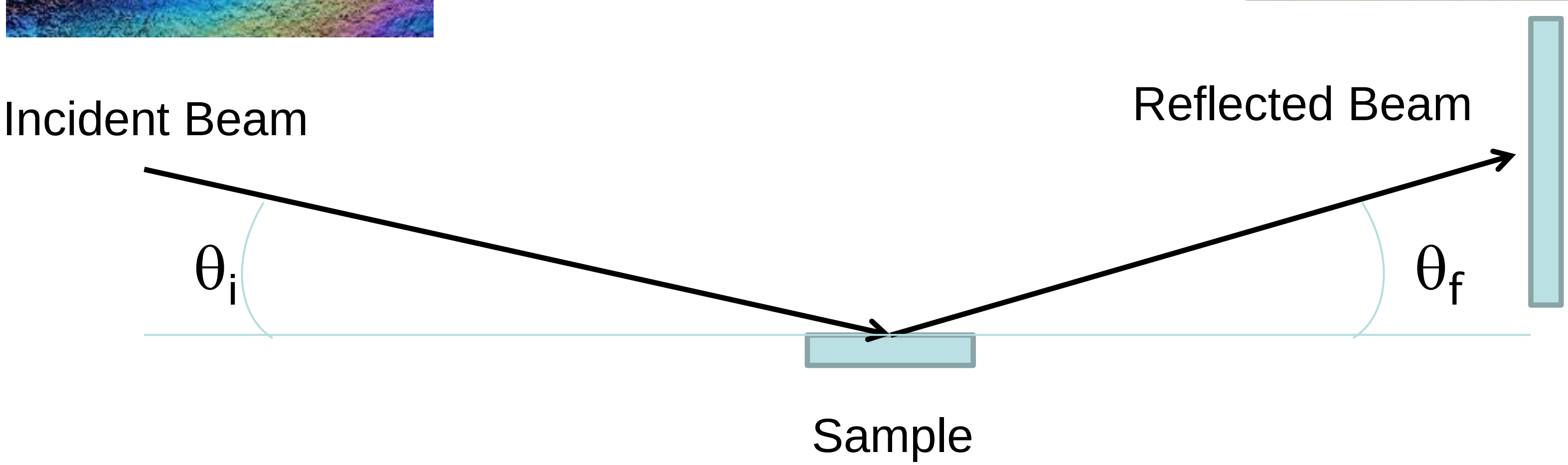
Specular Neutron Reflection

- Probe thin films at an interface which can be buried under neutron transparent material.
- Analogous effect to the rainbow generated by light reflecting from an oil film on water. Reflection and refracted beams are observed.
- $\theta_i=\theta_f$ for specular reflection which probes the direction perpendicular to the interface



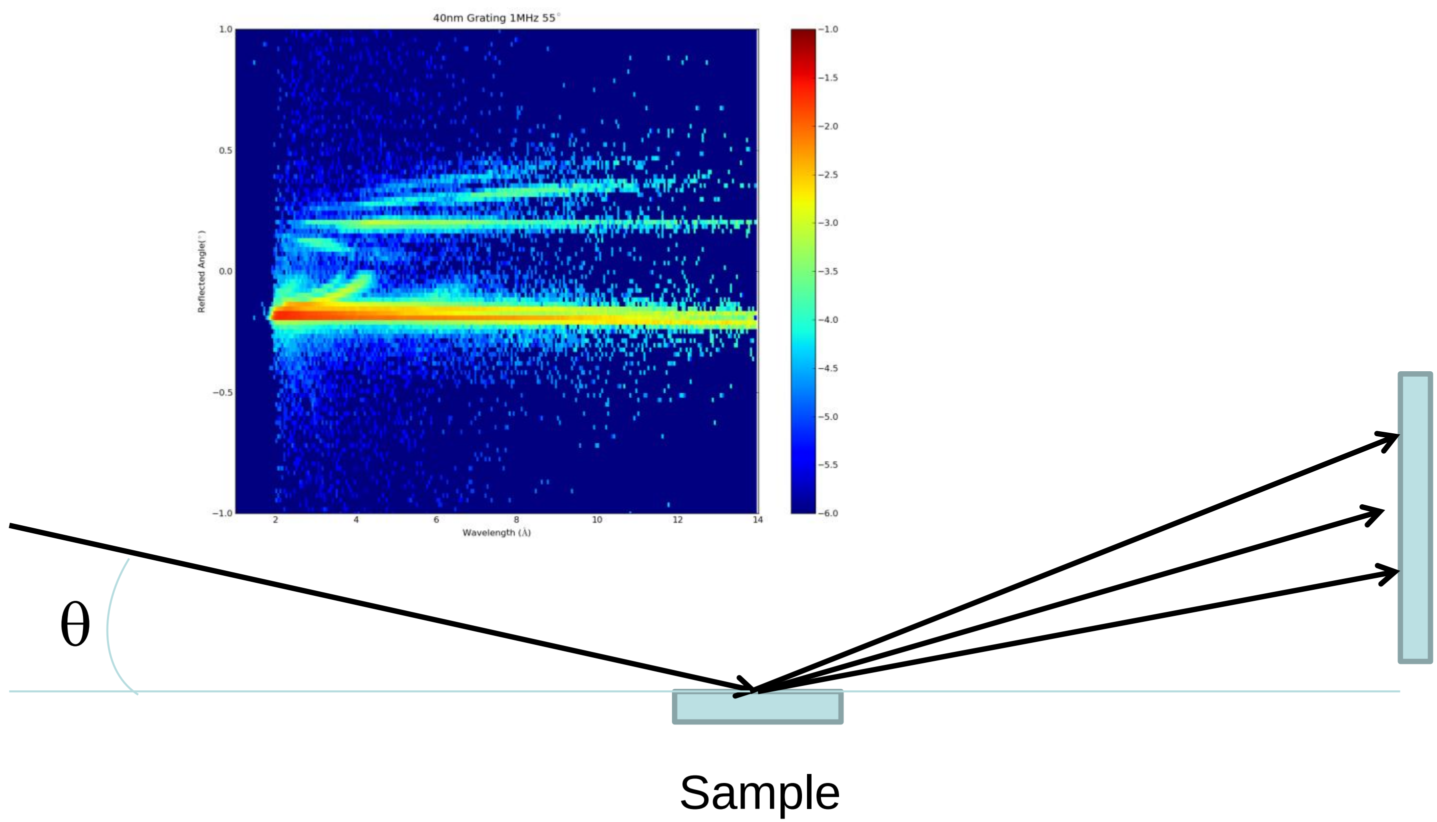
$$Q = \frac{4\pi \sin(\theta)}{\lambda}$$





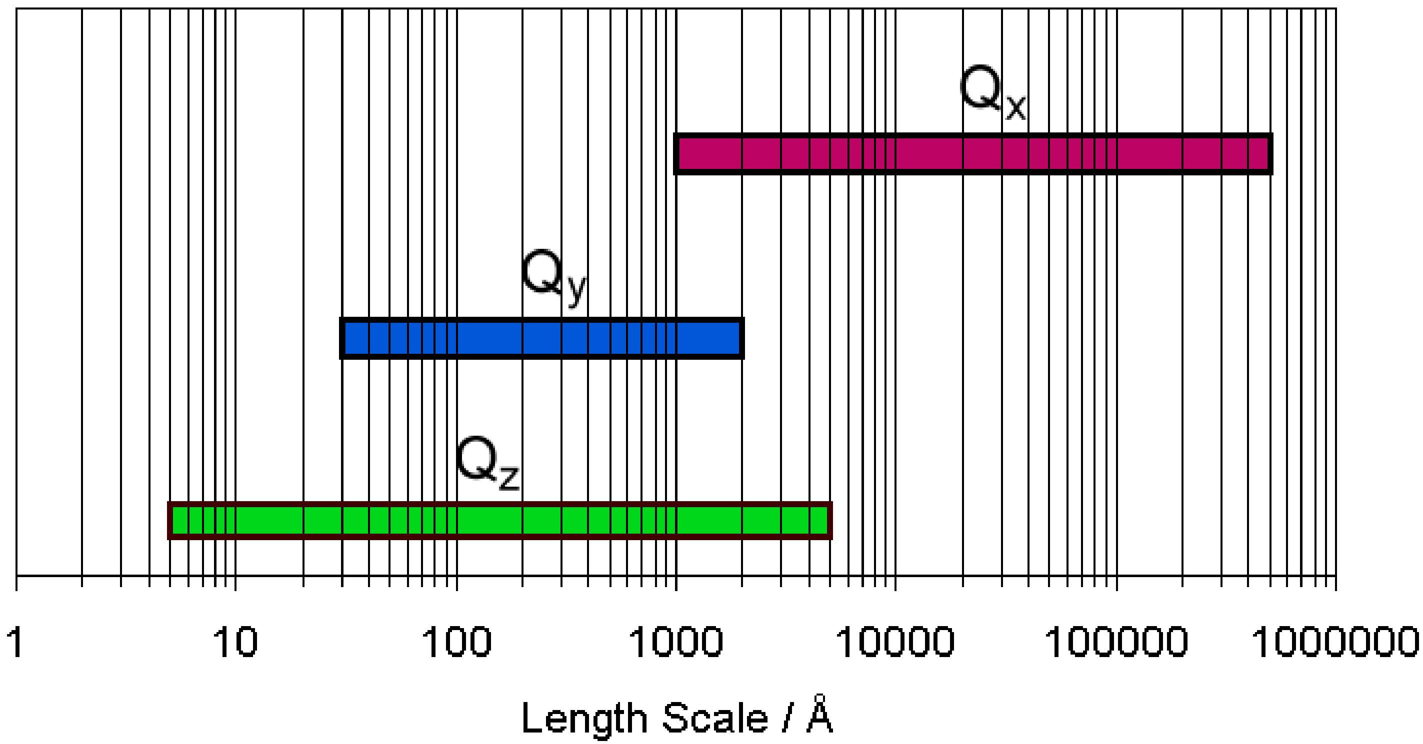
Off-Specular Scattering

- Probes both structure perpendicular to the interface and in the plane of the sample along the beam direction.
- McStas doesn’t have a sample to model this.

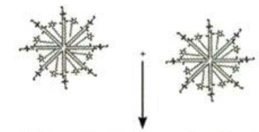


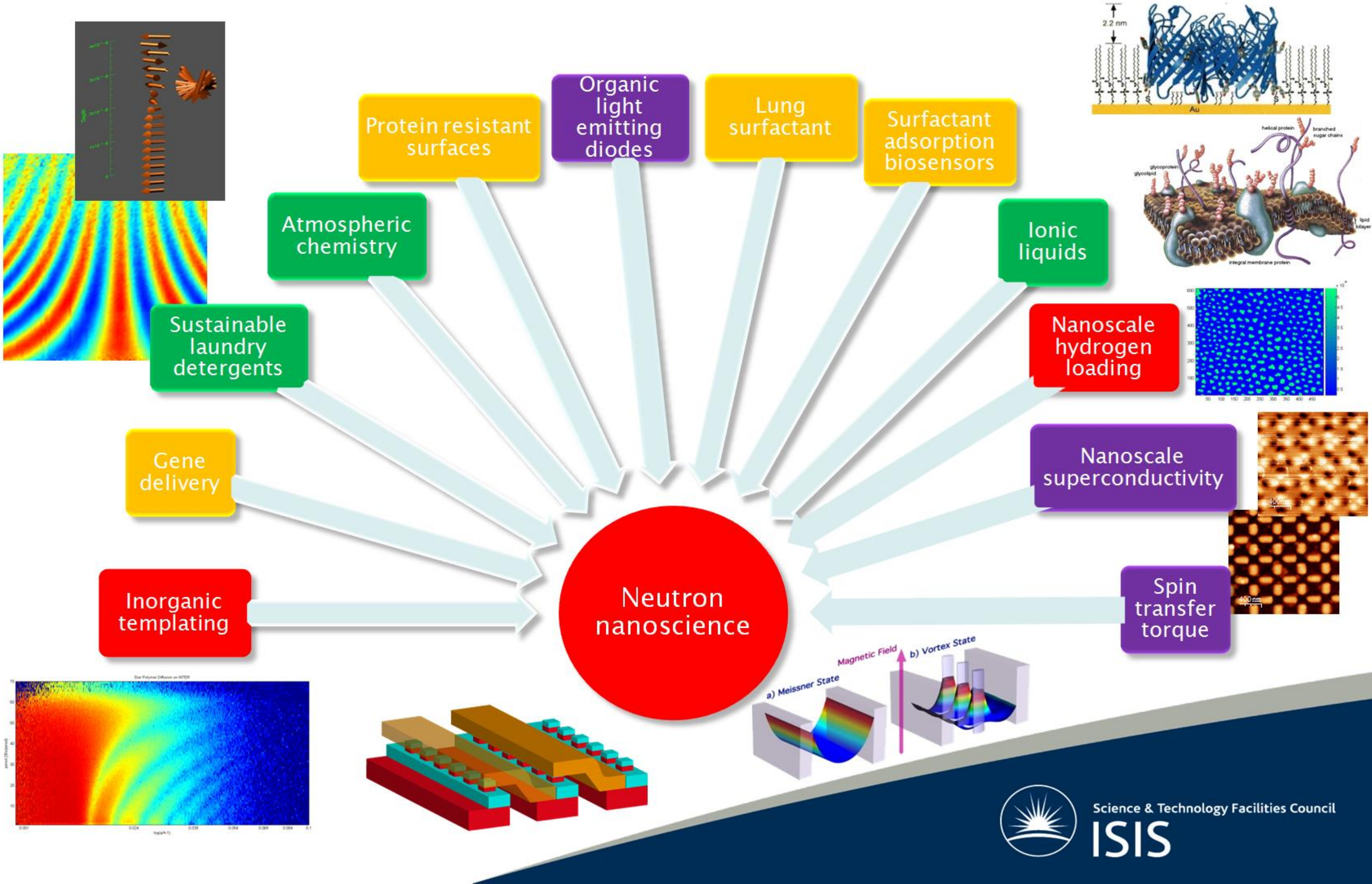
Reflectivity Length Scales

- Q_z Perpendicular to the interface
- Q_x In plane structure parallel to the beam
- Q_y In plane structure perpendicular to the beam



Neutron reflection science themes





Instrument Optimisation

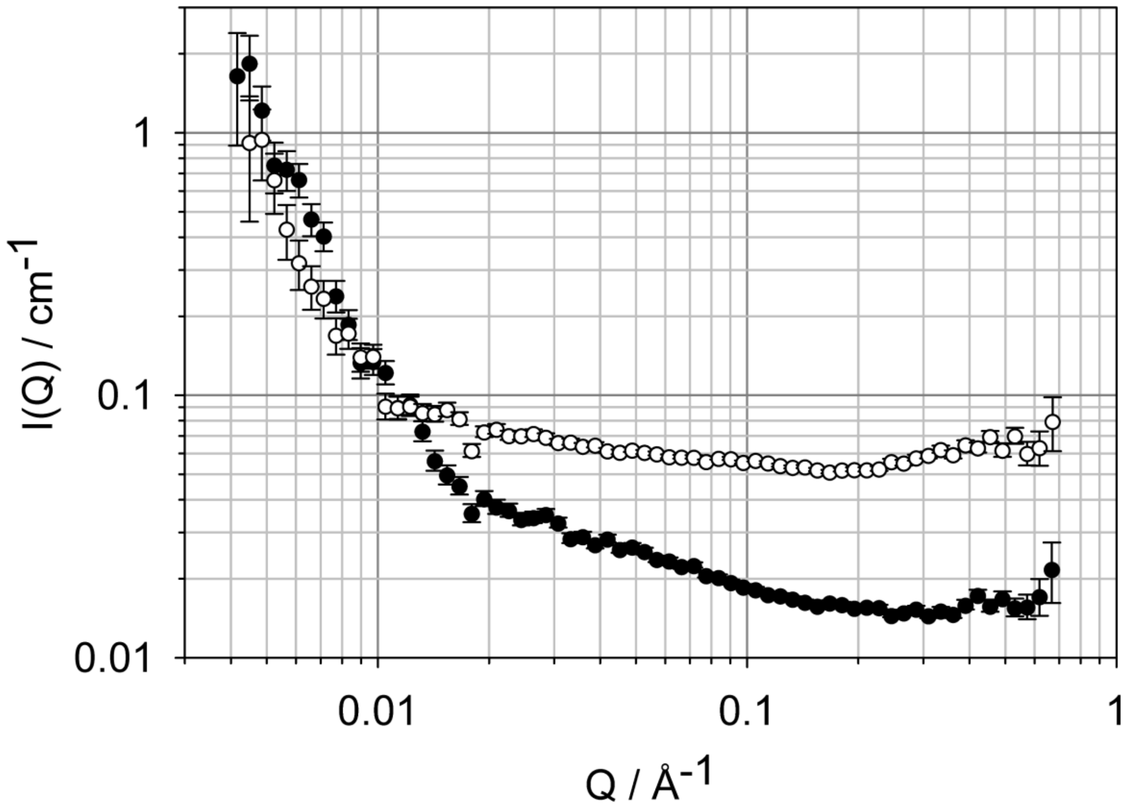
For NR and SANS the key to everything is background.

NR signals 10^{-7} or lower

SANS < $0.1 cm^{-1}$

McStas is <u>not</u> the best tool to determine this.

Larmor vs. SANS2D



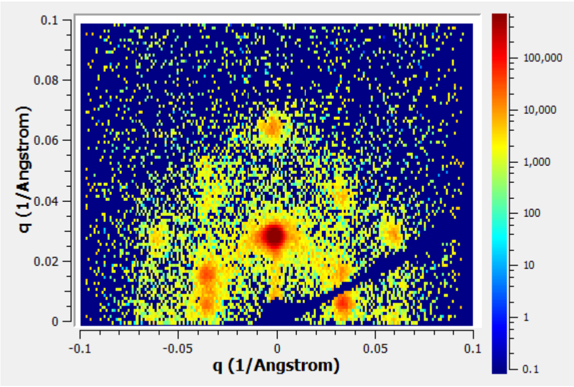
Larmor – Open circles
SANS2D – Filled circles

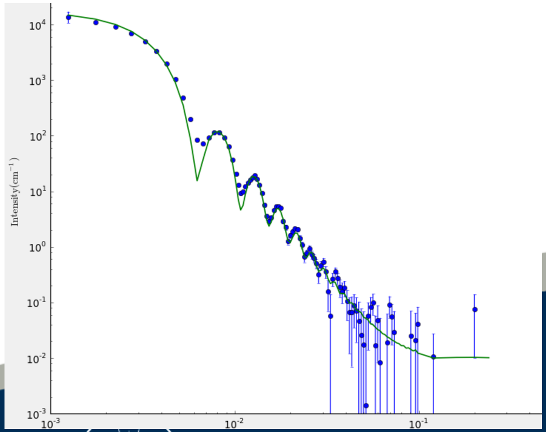
Empty instrument backgrounds scaled to absolute units.

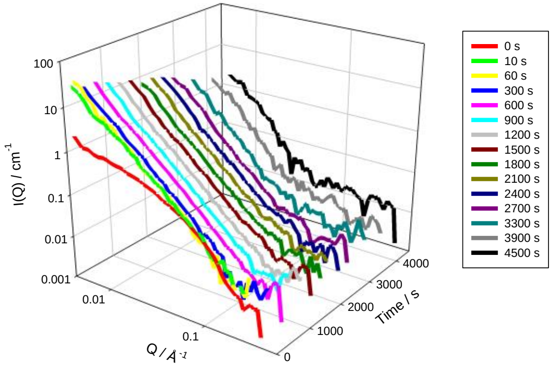
Factor of >3 background increase on Larmor. For weak signals (<0.1) a factor of 10 increase in counting time is needed to extract date with similar uncertainties

Science Focus

- SANS
  - Science focus determines instrument requirements and requires a science case. For example:
    - Broad simultaneous q range
    - Smallest qs
    - High flux with relaxed resolution
    - Polarisation
    - Complex sample environments
    - Grazing Incidence SANS

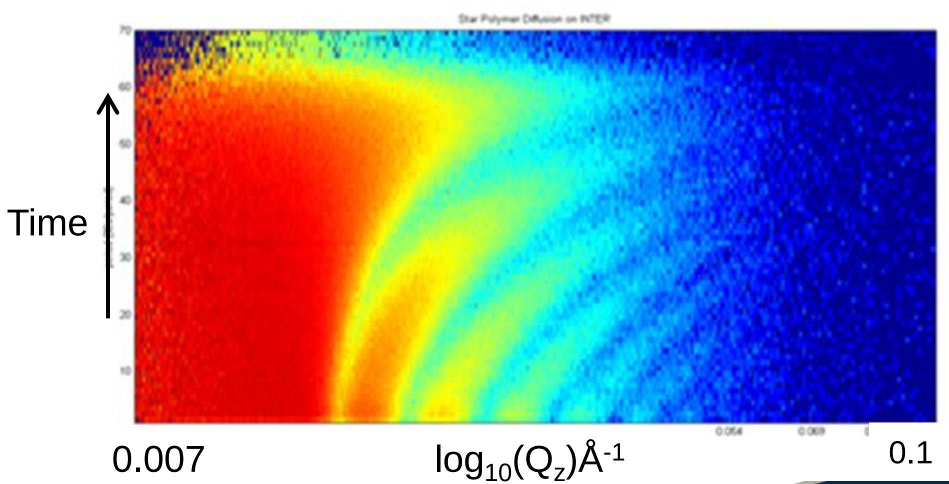


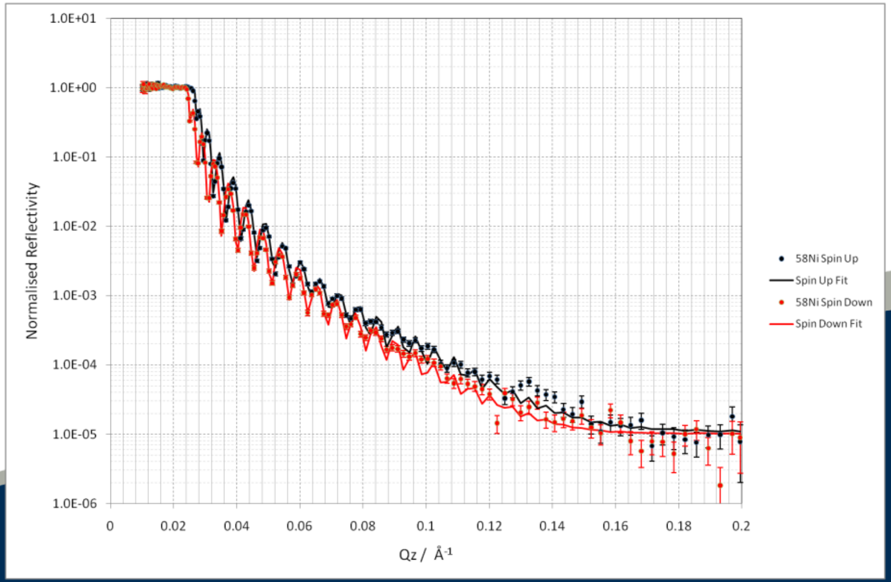




Science Focus

- NR
  - Science focus strongly determines instrument requirements
    - Broad simultaneous q range
    - Small samples
    - Specular reflection only
    - Polarisation
    - High flux with relaxed resolution
    - Complex sample environments



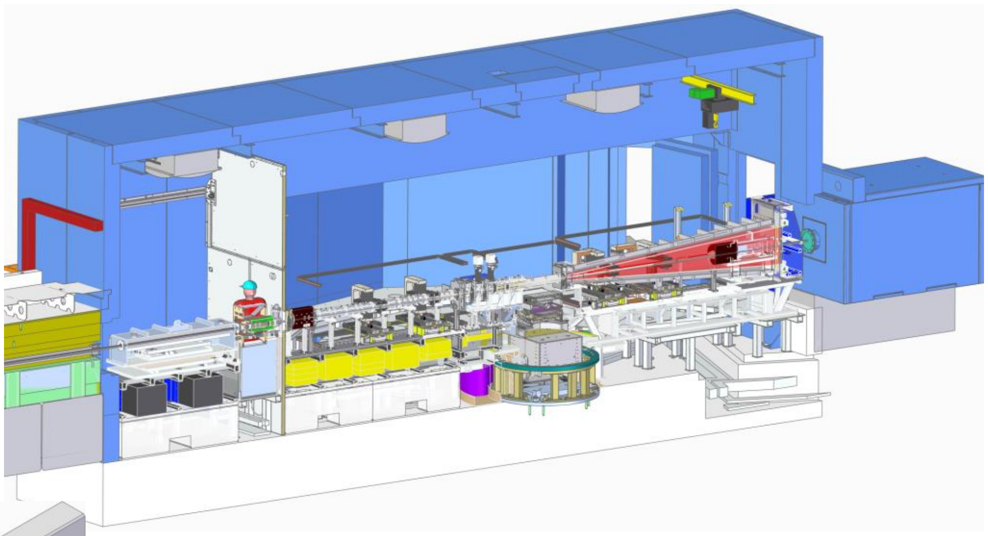


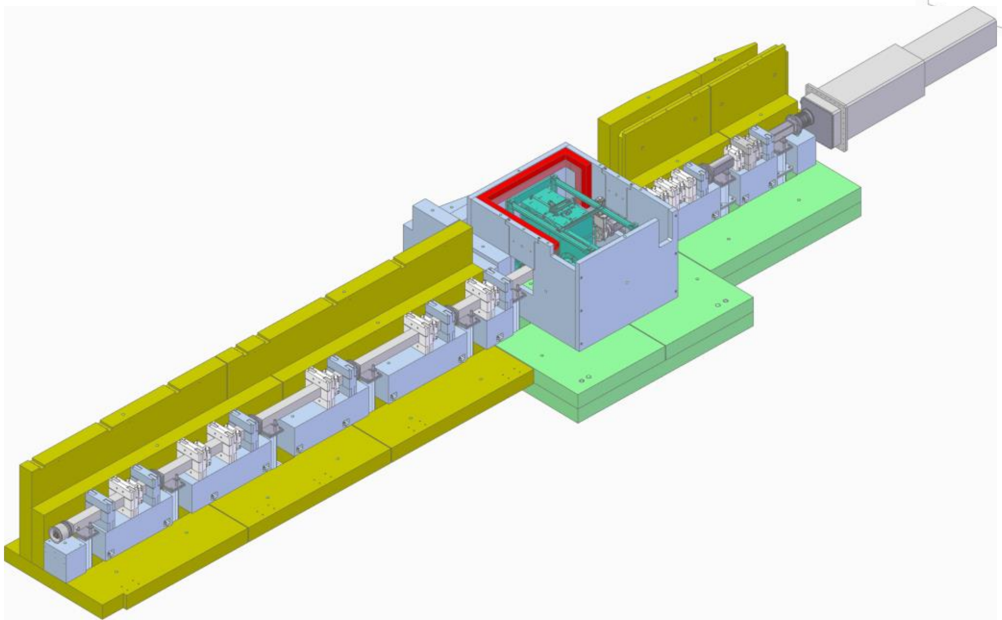
Groundwork

- Basic questions to be answer with spreadsheets
  - Q range required
  - Possible Wavelength Band
  - Chopper positioning
    - Need to know what is technically possible
  - Detector options
    - Pixel size and coverage

Groundwork 2

- Other limitations: Larmor
  - Many physical constraints

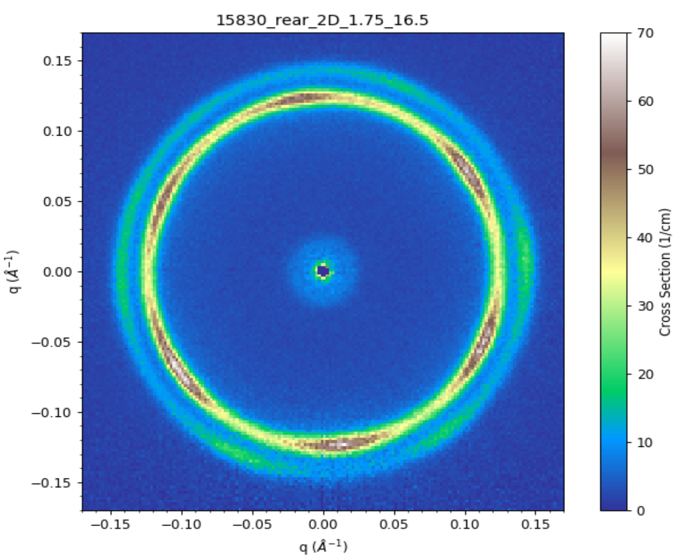


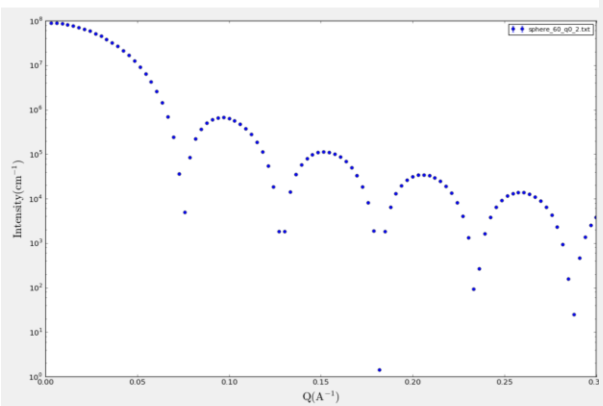


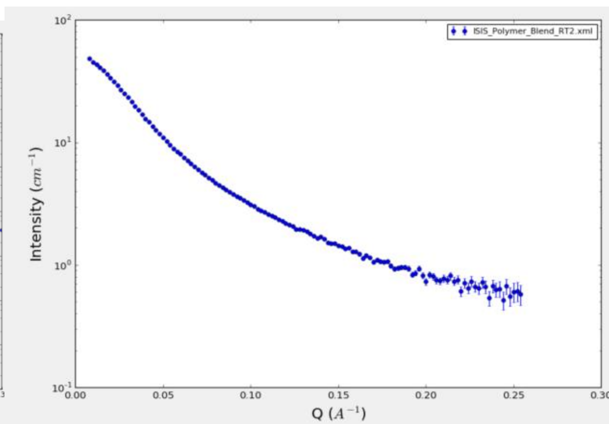
- Physical constraints strongly limited design options

Performance Metrics

- Unlikely to be just one
  - Flux on sample – a starting point only
  - Homogeneous phase space transport
  - Samples will be needed







NR Example

- Minimise the data collection time required to measure a 40x40mm sample consisting of a 15Å thick layer of SiO_2 on a silicon block against a pool of D_2O.
  - Background is ignored.
  - Q resolution must be considered
  - What q value is it important to reach?
  - What about thicker films?

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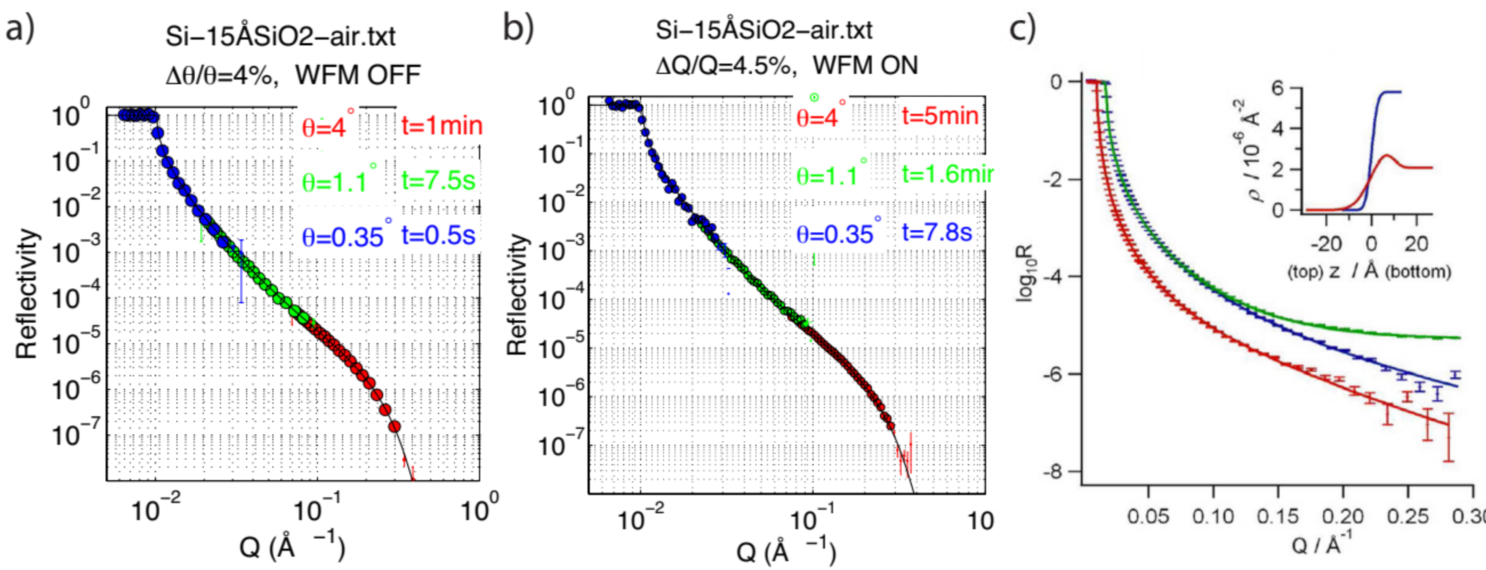
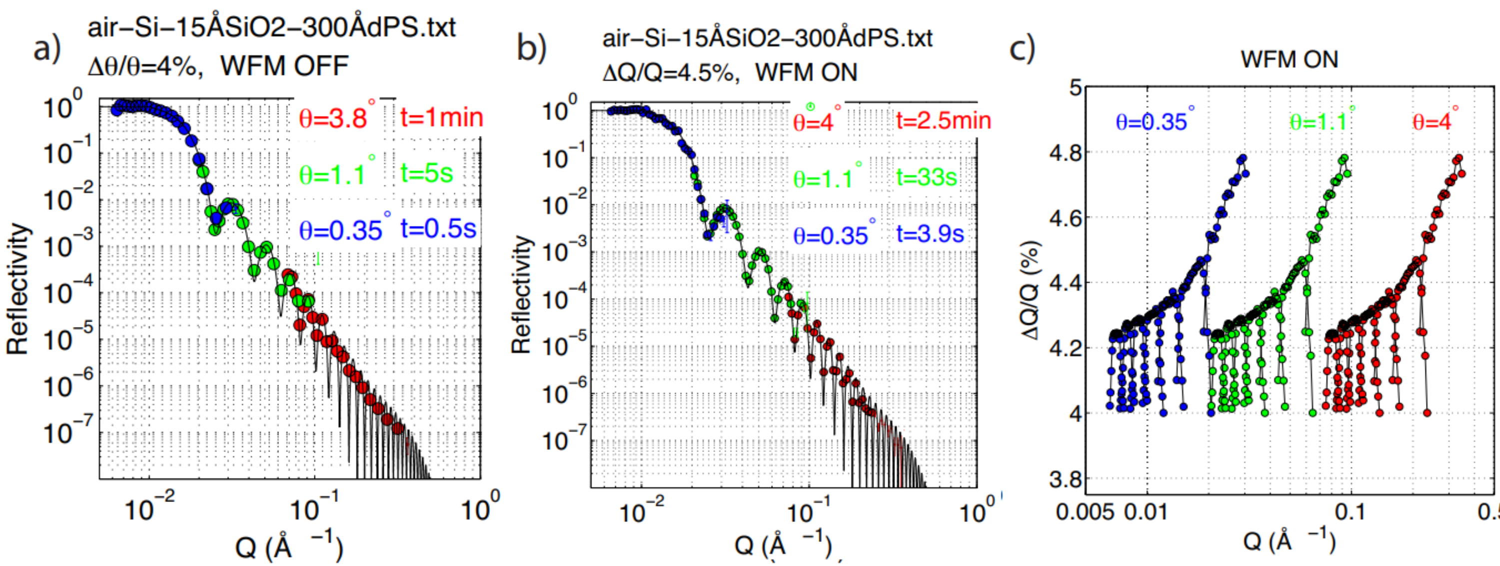


SiO_2 on Si
air



dPS on Si
air

McStas Samples

- SANS – There are lots:
  - The 3 most realistic/useful are
    - SANS_benchmark2
    - SasView_model
    - SANS_spheres2
- NR - Just one:
  - Multilayer_Sample

SANS_Benchmark2

COMPONENT sample = SANS_benchmark2(
xwidth=0.01,
yheight=0.01,
zthick=0.001,
model=model_nr, - model number to be picked from the list
dsdw_inc=0.0, - phenomenological incoherent background
sc_aim=1.0, - fraction to scatter (the rest transmit)
sans_aim=1.00, - fraction to SANS scatter the rest are incoherent
singlesp = 1.0) – Single or multiple scatter
AT (0, 0, 0.0) RELATIVE sampleMantid

Multilayer_Sample

COMPONENT samp1 = Multilayer_Sample(

xwidth = 0.05, - width of sample

zlength = 0.15, - length of sample along the beam

mu_inc=0.138, - incoherent scattering length

ythick=0.01, - thickness of the sample subphase

nlayer = 0, - number of layers

sldPar = {0.0,6.35e-6}, - list of layer scattering length densities

dPar = {0.0}, - list of layer thicknesses

sigmaPar = {5.0}, - list of interface roughnesses

target_index=1, - target to focus the incoherent scattering onto

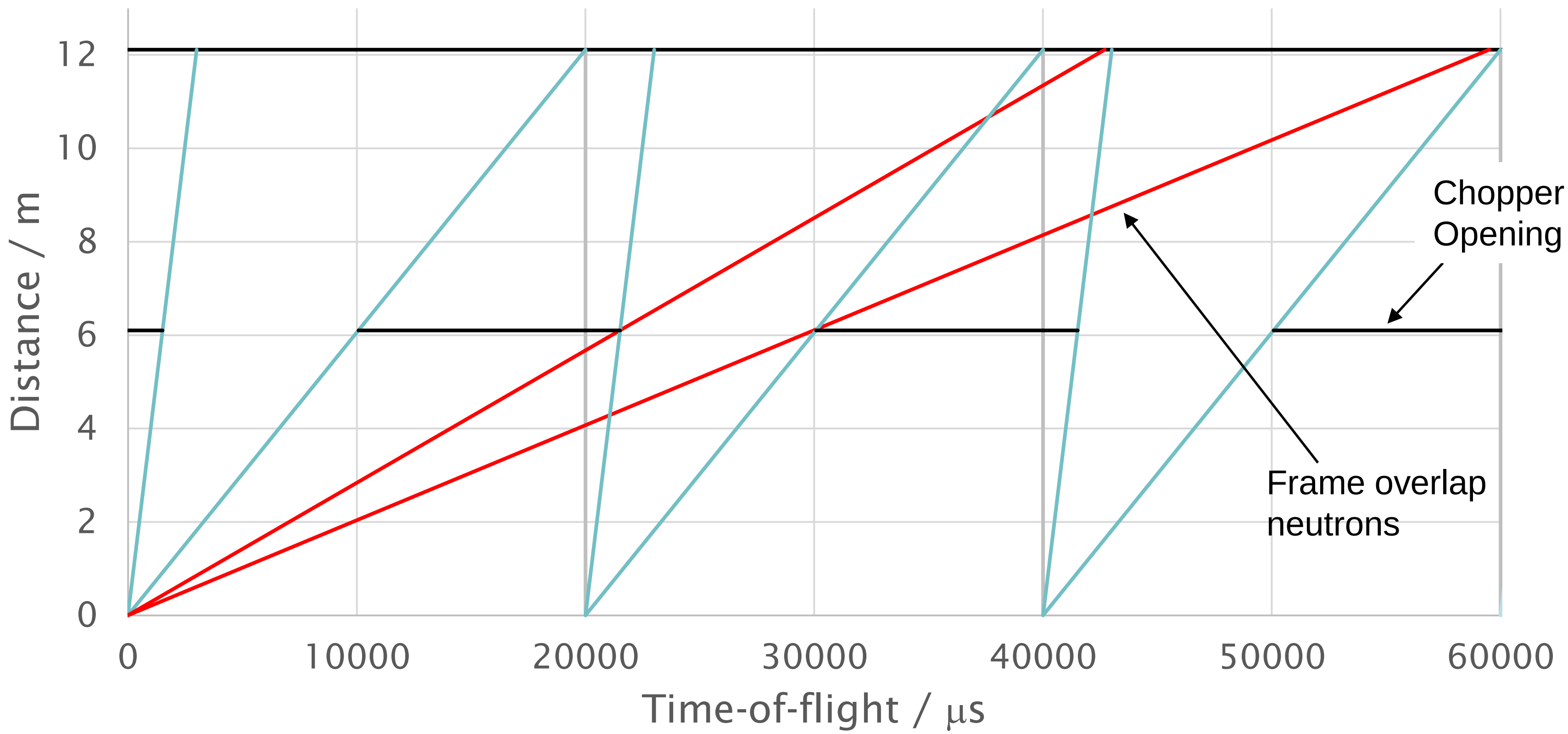
focus_xw=2*tend, - width of incoherent scattering focus

focus_yh=0.01, - height of incoherent scattering focus

frac_inc=FRAC) - fraction of neutrons to scatter incoherently

AT (0.0, spos*t15, spos) ABSOLUTE

Chopper Diagrams



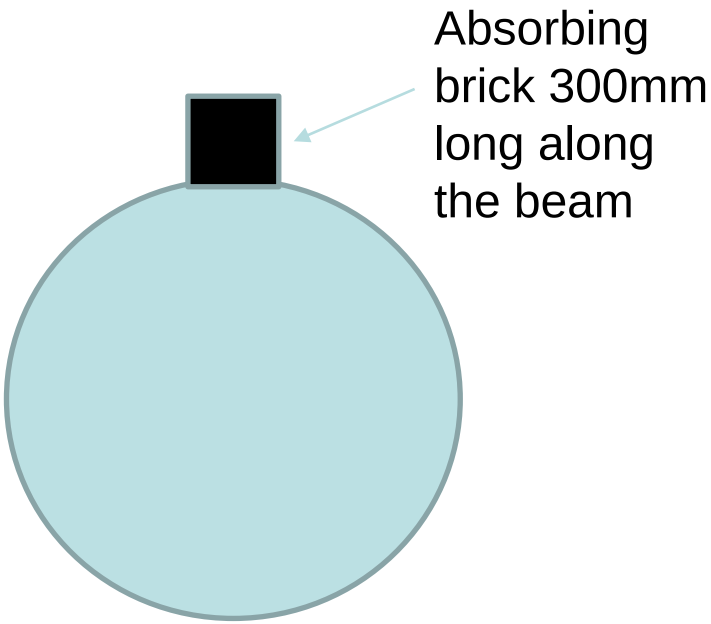
A simple spreadsheet will help with chopper positioning and will show where frame overlap problems will occur.

1Å neutron velocity = 3956.0339760560055 ms^{-1}

https://webapps.frm2.tum.de/neutroncalc/

T_0 Chopper

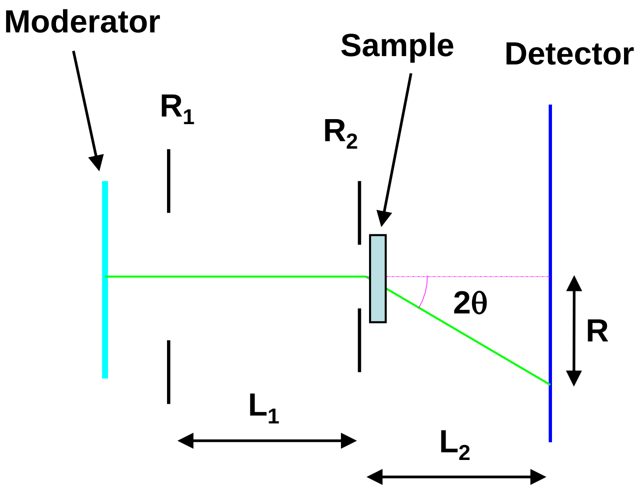
- Chopper to block the beam at time 0 when a flash of high energy neutrons passes down the beamline.



- How do you model this?

Q Resolution - SANS

- Mildner & Carptenter J.Appl.Cryst. 17(1984)249-256
- Assuming, small angles.
- Circular apertures, isotropic scattering, ΔR (Detector resolution) and Δλ are assumed to be rectangular distributions not Gaussians.

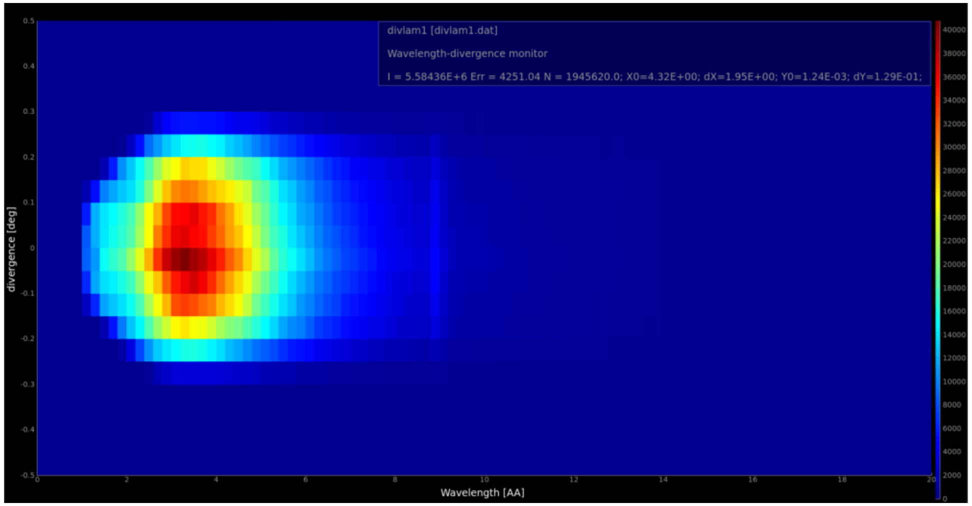


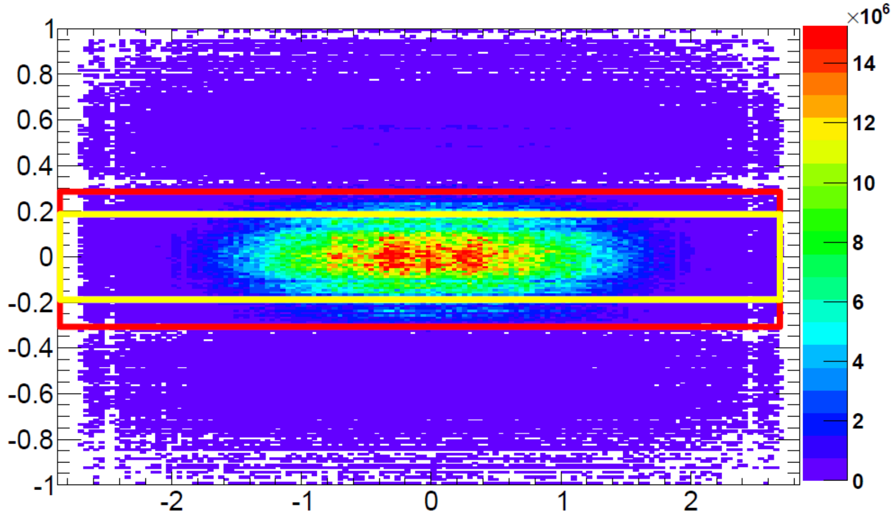
- Optimal SANS configuration when $L_1=L_2$ and $R_1=2R_2$
- Weak constraint: Changing L_1 and L_2 allows the wavelength band be changed

$$\left(\frac{\sigma_Q}{Q}\right)^2 = \left(\frac{R_1 L_2}{2RL_1}\right)^2 + \left(\frac{R_2(L_1+L_2)}{2RL_1}\right)^2 + \frac{1}{12}\left(\frac{\Delta R}{R}\right)^2 + \frac{1}{12}\left(\frac{\Delta\lambda}{\lambda}\right)^2$$

Phase Space

- Homogeneous illumination of the sample is important for normalisation in both NR and SANS
  - Add a PSD monitor after A2 to probe the beam shape before the sample
  - Add 2 divergence monitors to probe the divergence transported to the sample in both X and Y





ISIS Moderator Component

- The new component and moderator files for many of the ISIS instruments can be found on the NMIDG webpage
- Follow the link [Moderator files for use with McStas]
- Download Commodus_I.comp and then explore the Baseline and TS1upgrade folders to see if the a suitable file exists. The TS1instruments should all be there but only a few TS2 instruments have been added

- If not then the existing files distributed with McStas will work but will not have been updated to reflect the existing state of the moderators. If you want an updated file to be produced then you will need to ask the neutronics group to produce one.

Using Commodus_I

```
COMPONENT sourceMantid = Commodus_I(
Face="Larmor_Base.mcstas", - data file in the folder with the .instr
E0 = E_min, - Minimum neutron energy
E1 = E_max, - Maximum neutron energy
modXsize = 0.083, - moderator width
modZsize = 0.033, - moderator height
xw = 0.03, - target window width
yh = 0.03,  - target window height
dist = 3.7)  - distance to target window
AT (0.0, 0.0, 0.0) RELATIVE Origin
```

Add this to the INITIALIZE section or E0=…..

```
E_max=81.8047/(lmin*lmin);
E_min=81.8047/(lmax*lmax);
```

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Concluding Comments

- Optimisation of an instrument is extremely complicated.
  - Define your metrics in discussion with others
  - Accept the fact that there will be a lot of compromises to be made.
  - Don’t forget about misalignments.

Exercises SANS

- SANS
  - Download the SANS2D instrument file from Github https://github.com/McStasMcXtrace/McCode/tree/master/mcstas-comps/examples
  - Compile and launch the trace so you can see what the instrument looks like.
  - Identify the key components of the instrument
    - Why is there a bender?
    - Why is the guide so small?
    - Why is the m value of the guide sections so low?
  - Modify the instrument to explore the incident divergence before the sample
  - Add a beamstop with a radius of 30mm to block the direct beam from hitting the detector
  - Modify the instrument to change the L1 and L2 and explore how this effects the q range
  - Modify the m value of the guides to see how this effects the incident flux
  - Add a dummy guide to explore the effect of gravity

Exercises NR

- NR
  - Download the CRISP instrument file from Github https://github.com/McStasMcXtrace/McCode/tree/master/mcstas-comps/examples
  - Modify the file to use the new moderator component and compare the results with the version distributed with McStas. Take care to read the instructions detailing how to calculate the flux.
  - Modify the sample component to add layers to produce fringes.
  - Modify the instrument to allow the sample angle to be scanned.
  - Write a linear TOF detector or use monitor_ND to write one.
  - Add the choppers and expore frame overlap effects