Introduction to the Disk Chopper Spectrometer (DCS)

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This presentation

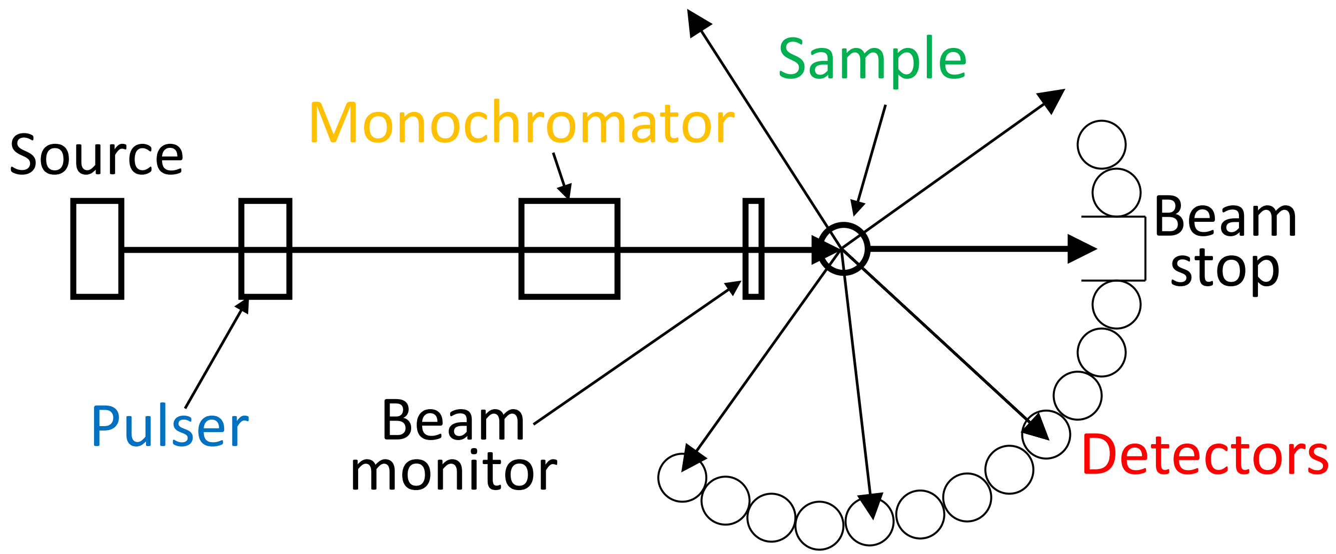
- DCS instrument layout
- How DCS works
- How to perform an experiment
- What DCS data look like

What is DCS?

- A neutron spectrometer based on
  - Low-energy reactor-based neutron source
  - Tunable incident energy and resolution
  - Multi-detector subtending wide solid angle
- Used to interrogate excitations in materials
- Wide variety of science
  - Soft matter
  - Liquids
  - Energy materials
  - Quantum materials

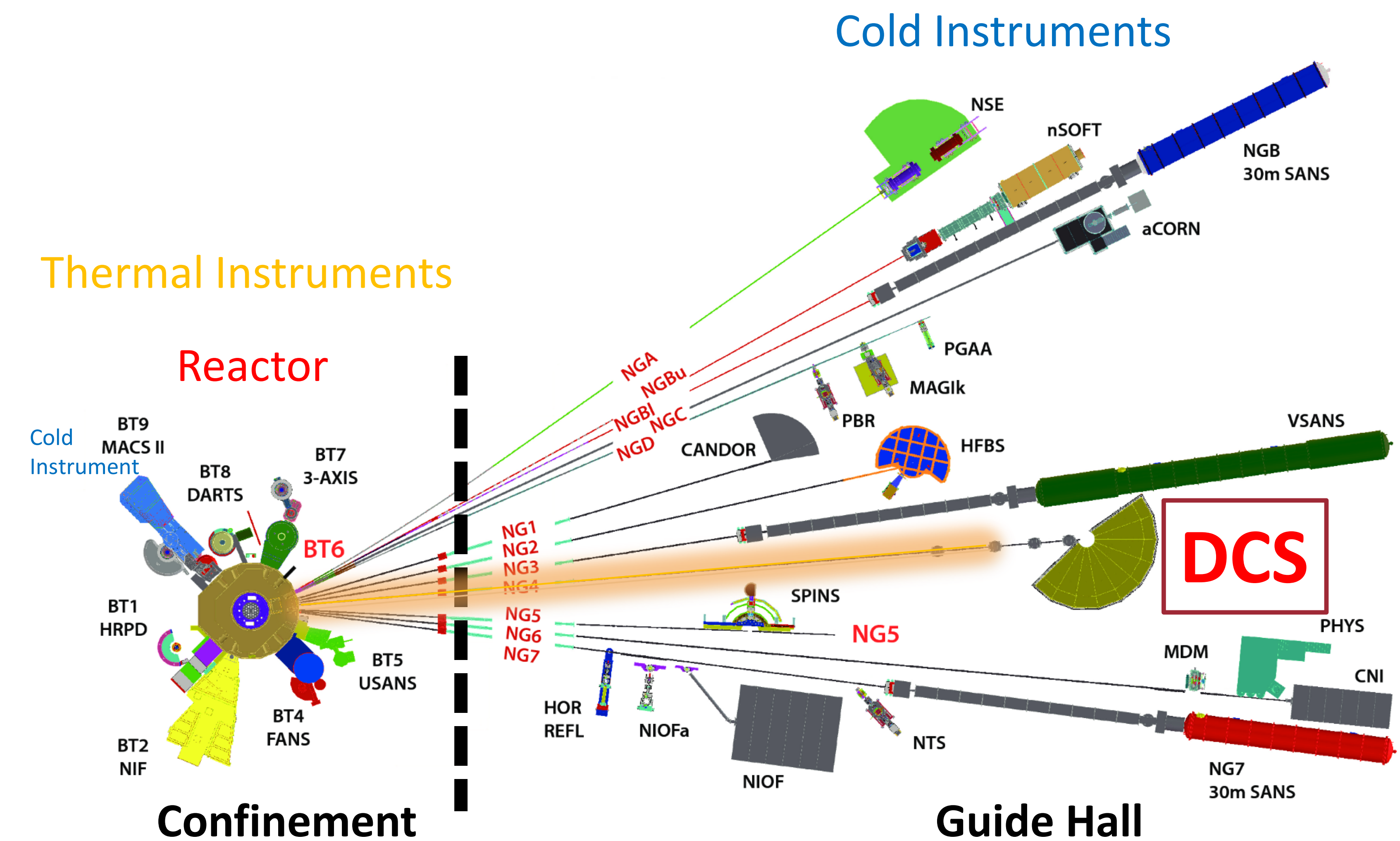
General Plan

Time-of-flight principle of operation

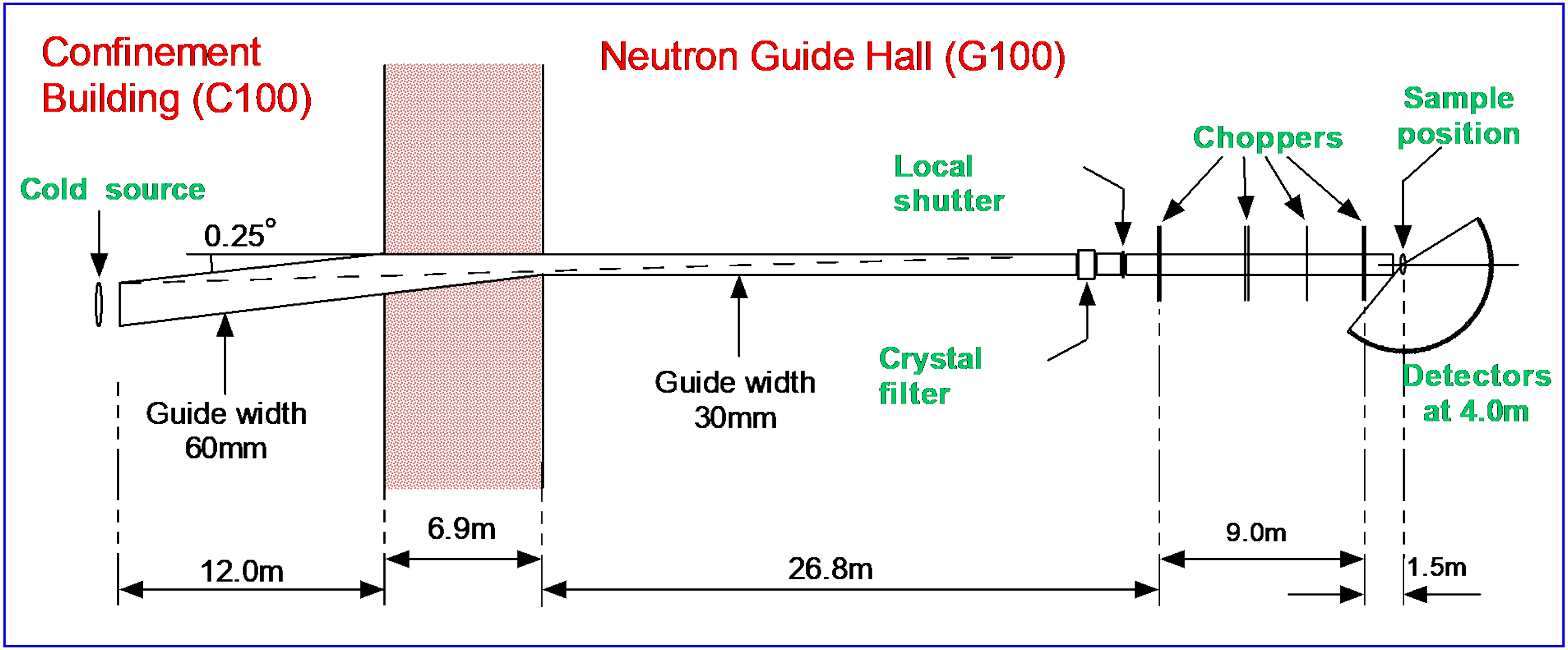


1. Neutrons from the source are pulsed and monochromated
   *Set *incoming* energy, direction, and time
2. Monochromatic bursts of neutrons strike the sample
3. Some of the neutrons are scattered, and some of the scattered neutrons are counted in the detectors
   *Measure *outgoing* energy, direction, and time

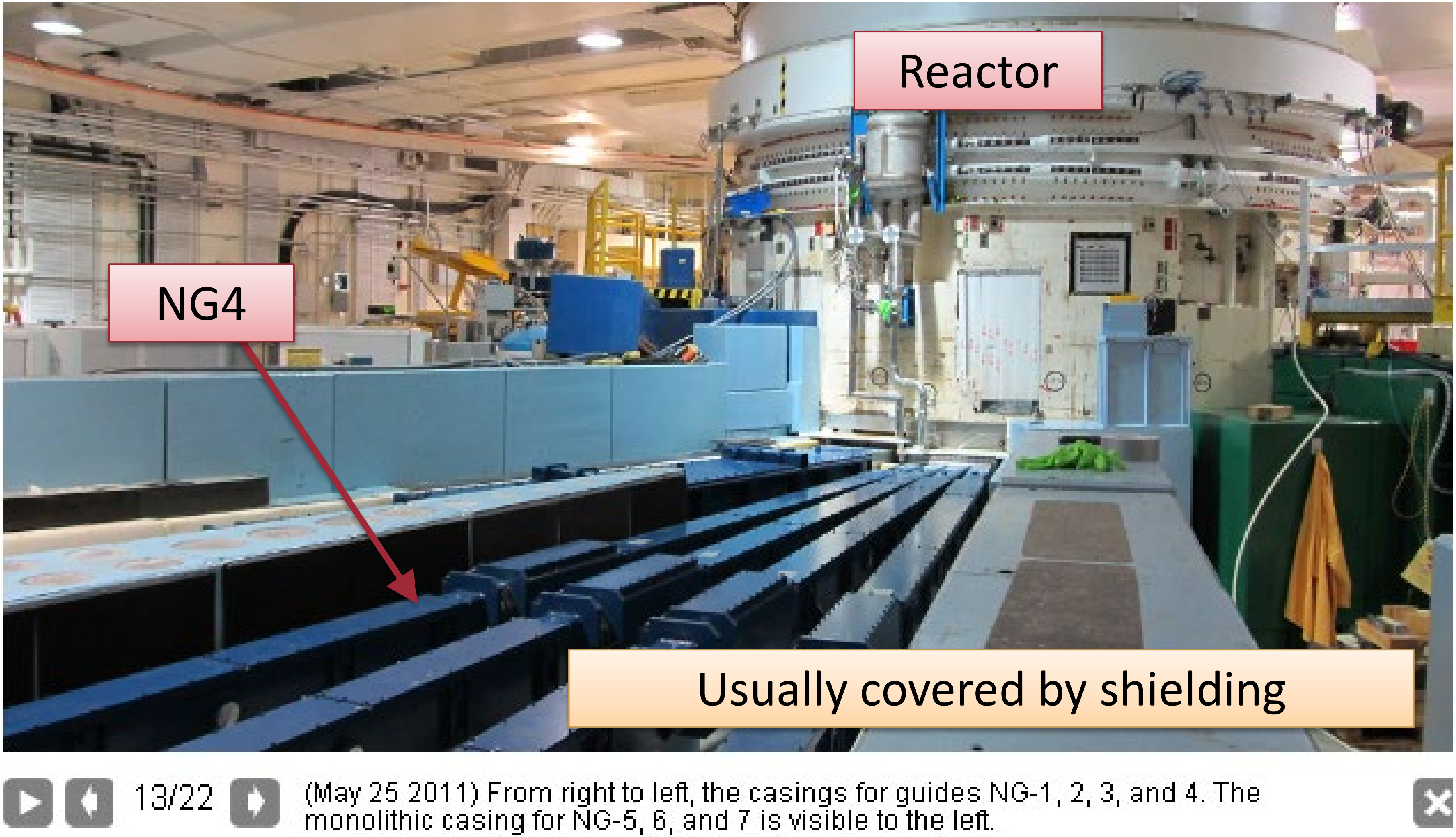
NCNR instrument layout



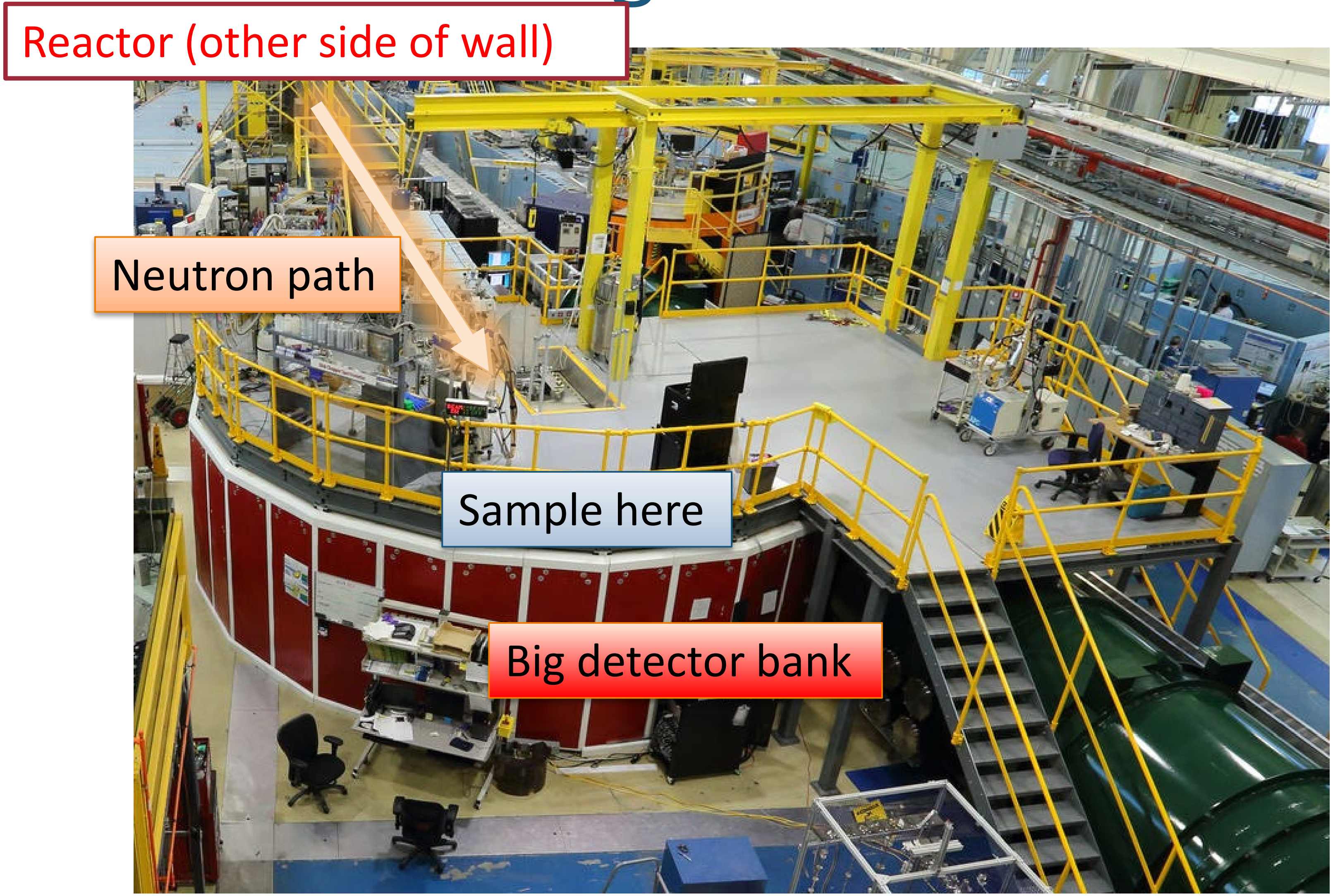
DCS plan view



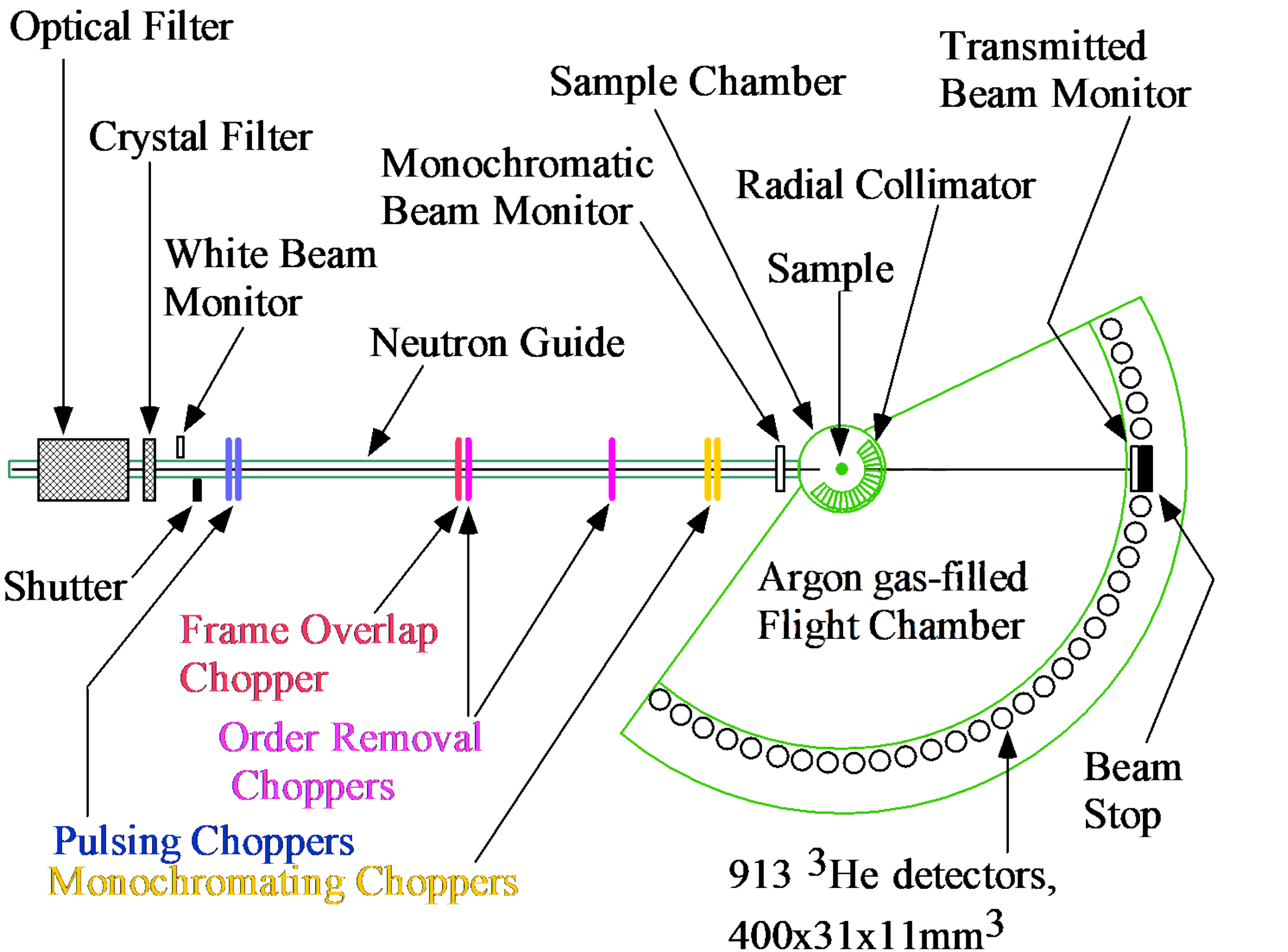
Neutron guides in the confinement building



DCS looking toward reactor

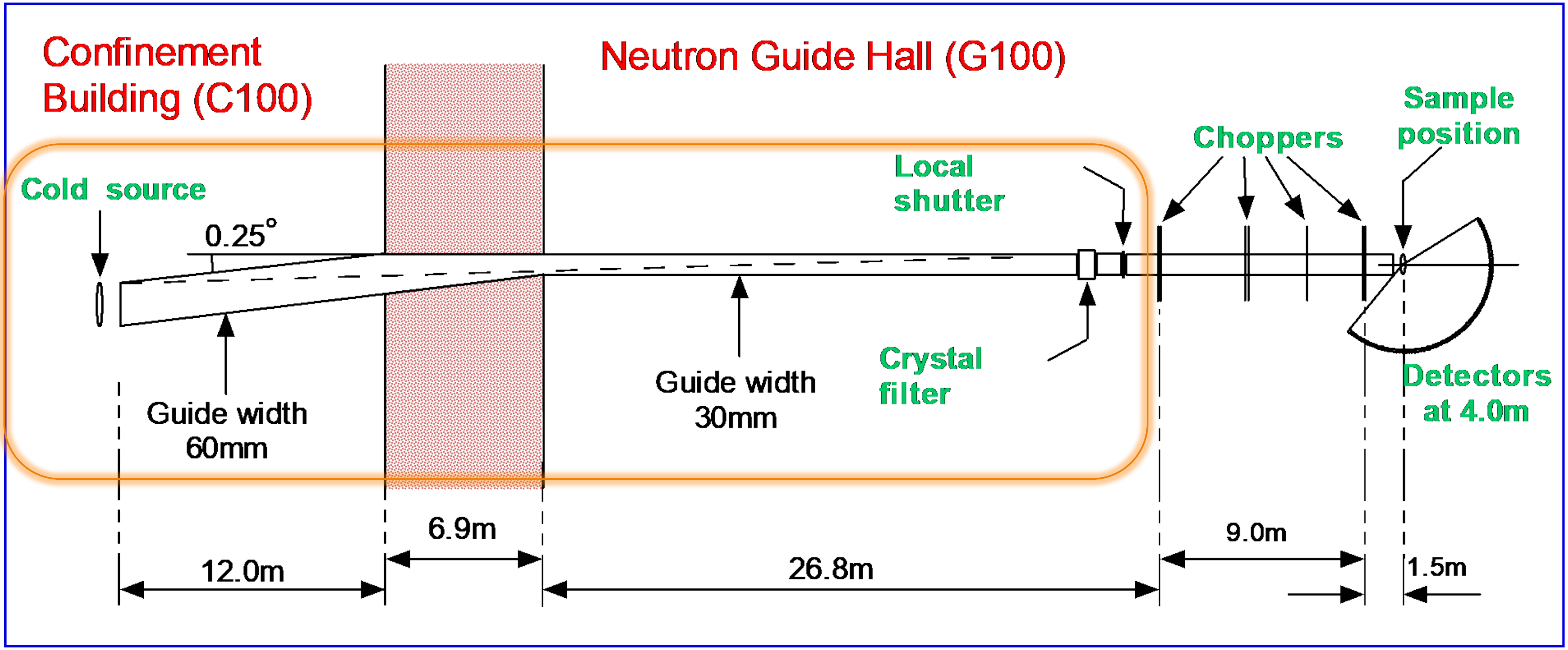


The Disk Chopper Spectrometer - schematic



Neutron guide

DCS plan view



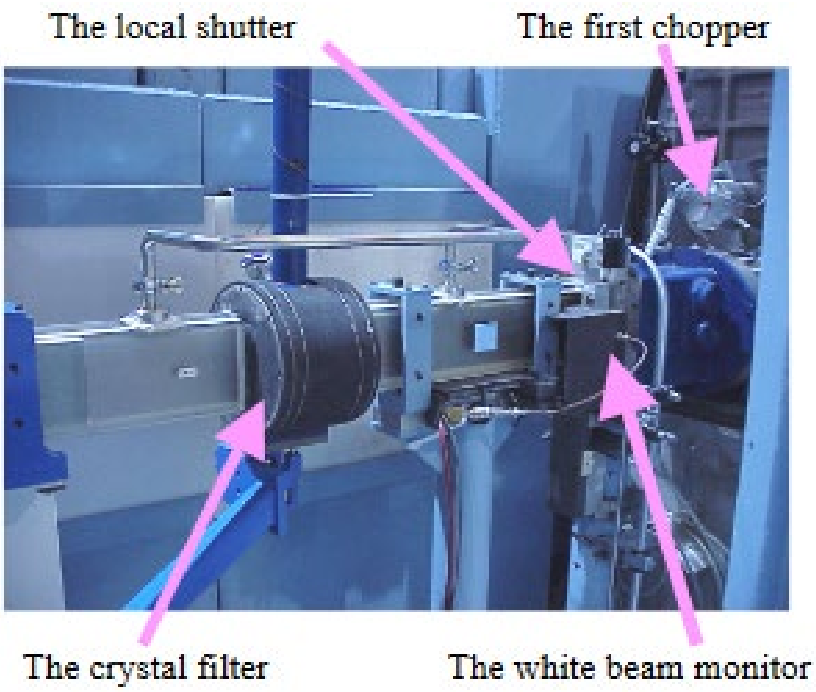
Pre-shutter guide

The guide, looking toward the cold source

- Neutron "pipe"
- No line of sight between cold source and local shutter
- Guide tapers over 7m
  – Confinement: 60mm (w) x 150mm
  – Guide hall: 30mm (w) x 100 mm
  – Turns 0.25° w.r.t. original direction
- Guide coatings:
  – Top, bottom: "$2\theta_c$" supermirror
  – Side: ^{58}Ni-equivalent (Ni + 6 Ni-Ti bilayers)

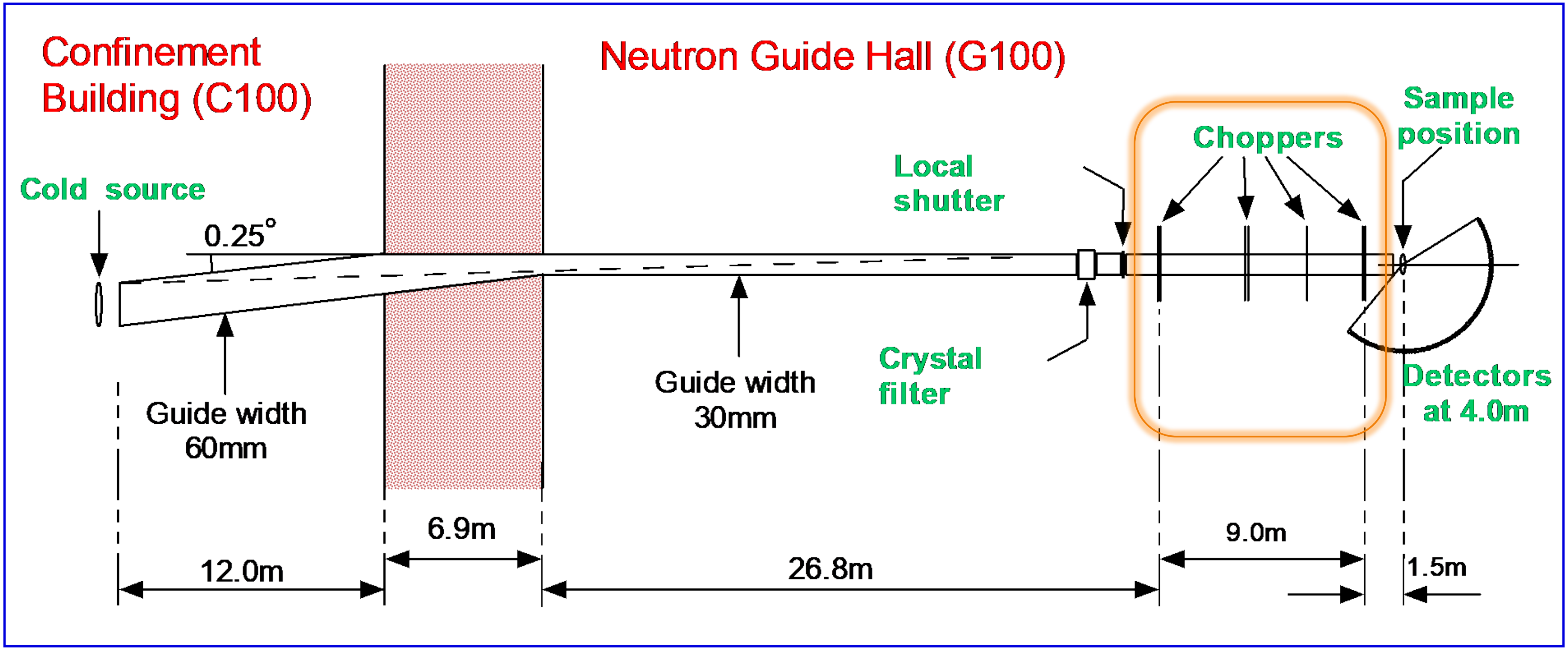
Before the choppers

- Crystal filter:
  - 100mm thick ZYH ("filter grade") pyrolytic graphite, c-axis oriented
  - cooled to 77K
- Local shutter
  - Beam "on/off"
  - 3mm LiF
  - 38.1mm heavimet (mostly tungsten)
- White beam monitor
  - when shutter is open
  - views entrance window of the post-chopper guide

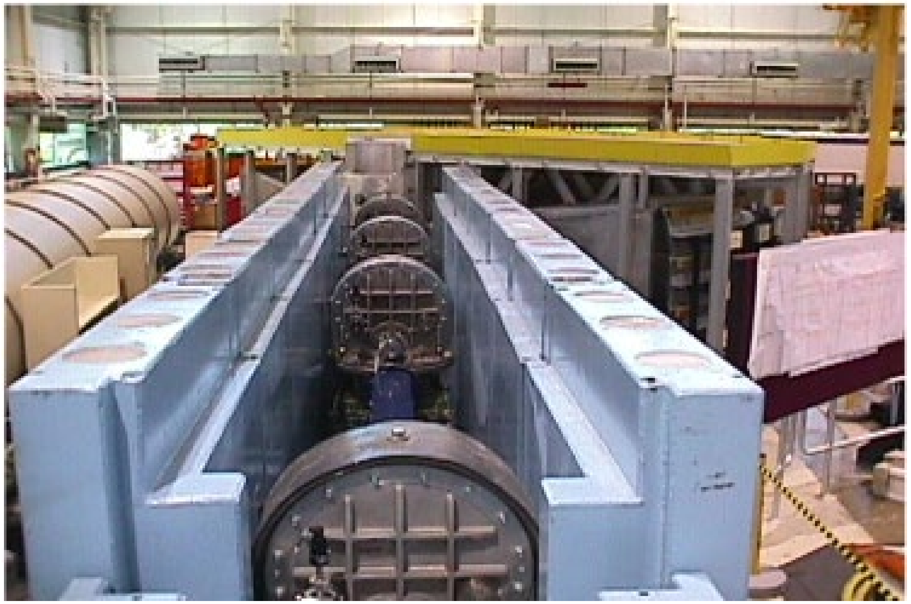


Choppers

DCS plan view



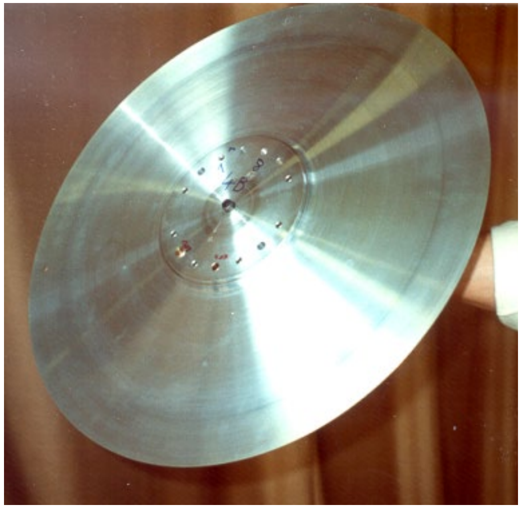
Guide through the choppers

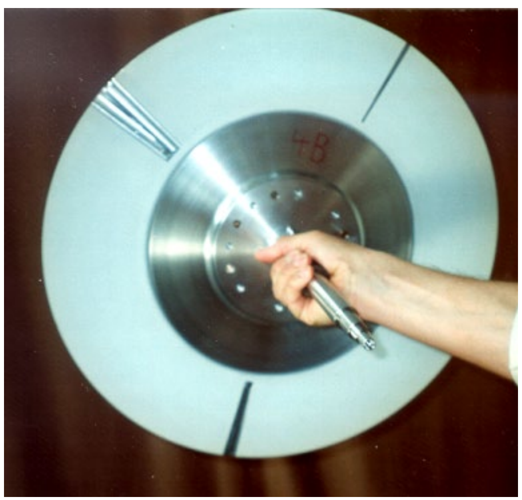


Chopper housings, looking toward the DCS instrument (under construction)

- 30mm (w) x 100mm (h)
- 20mm cutouts for choppers
- Guide + chopper housings share common vacuum $\leq 10^{-3}$ mTorr

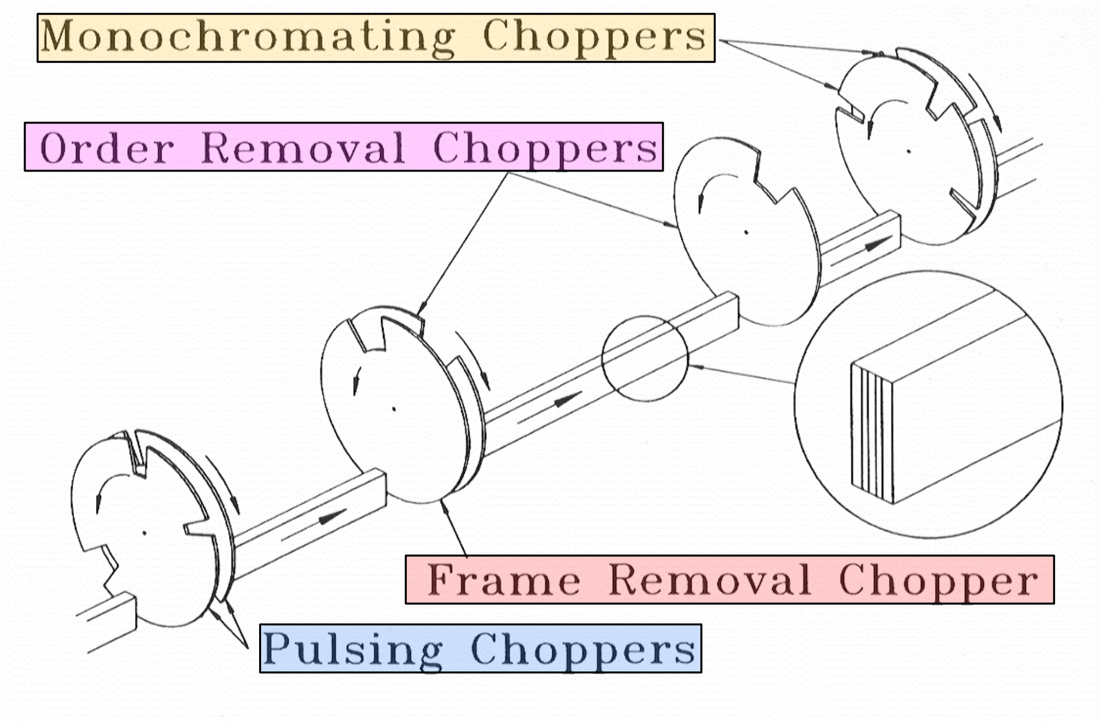
Choppers





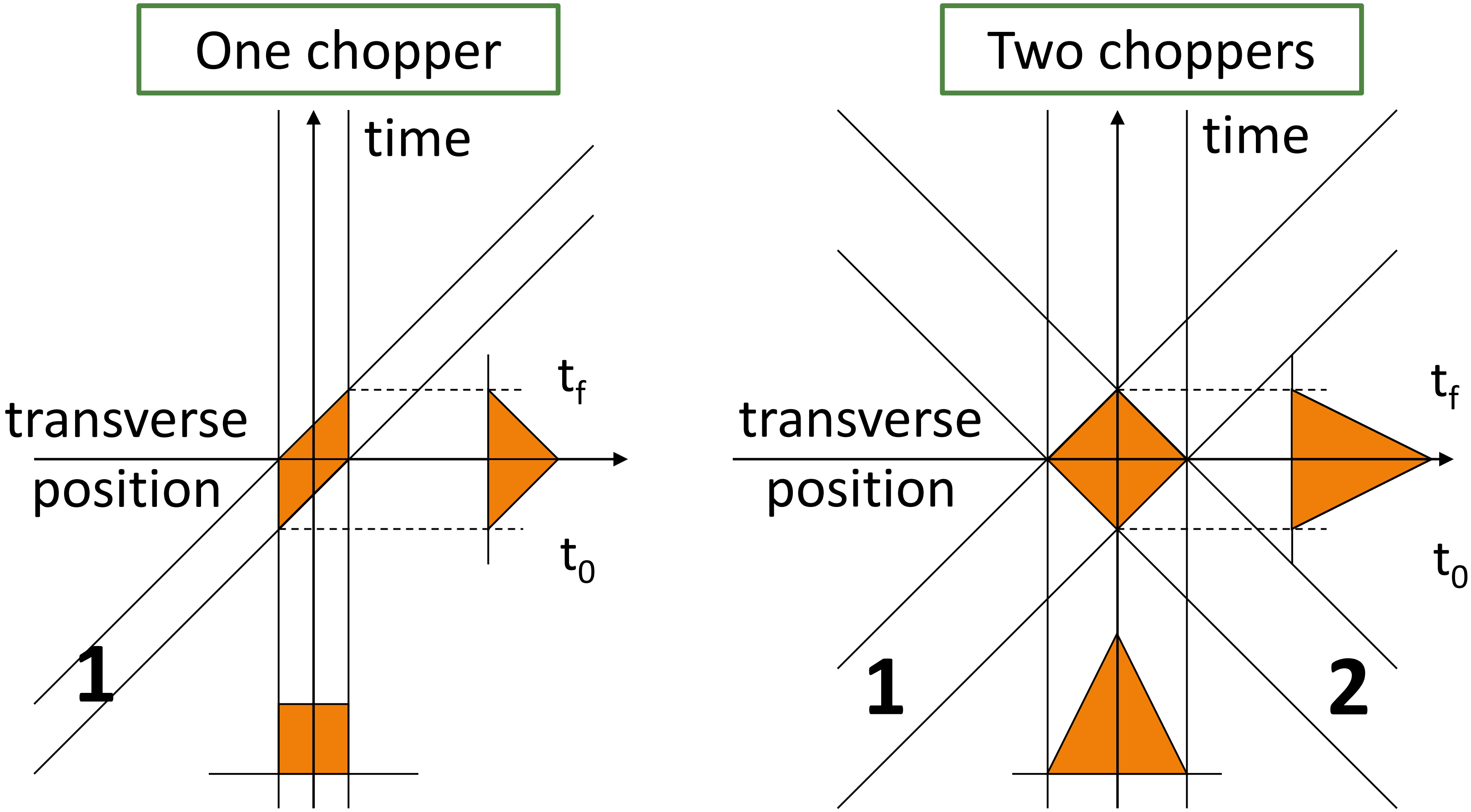
- High strength Al alloy
  - 580 mm diameter disk
  - mean thickness < 2 mm
  - Max spin: 20,000 rpm
- Neutron absorber
  - r ≥ 175mm
  - plasma-coated Gd_2O_3
- Windows
  - Gaps in coating
  - Angular widths: 1.35° - 20°
  - Pulse width / resolution

Chopper configuration



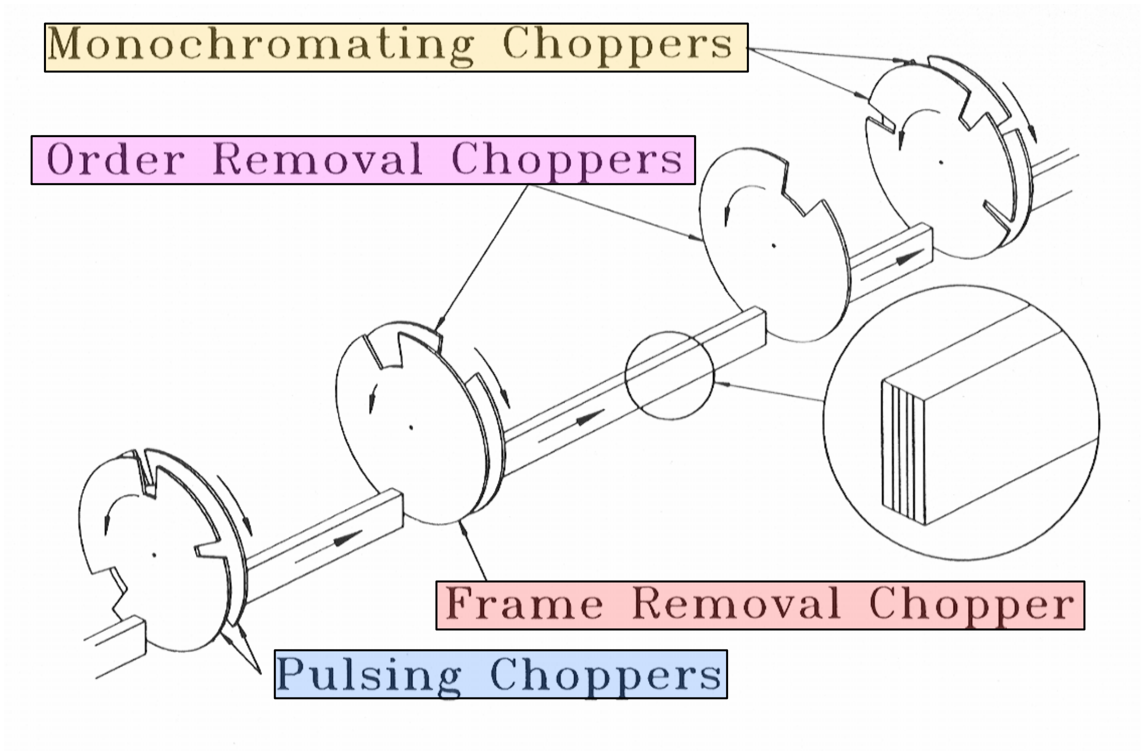
1. ***Pulsing*** and ***monochromating*** **counter-rotating**, **paired** choppers control pulse width, i.e., energy resolution (Normally 20,000 rpm)
2. ***Order removal*** choppers remove contaminants (Also 20,000 rpm)
3. ***Frame removal*** chopper to mitigate frame overlap (Lower speed: 20,000/m or 20,000(m-1)/m rpm)

Counter-rotating choppers

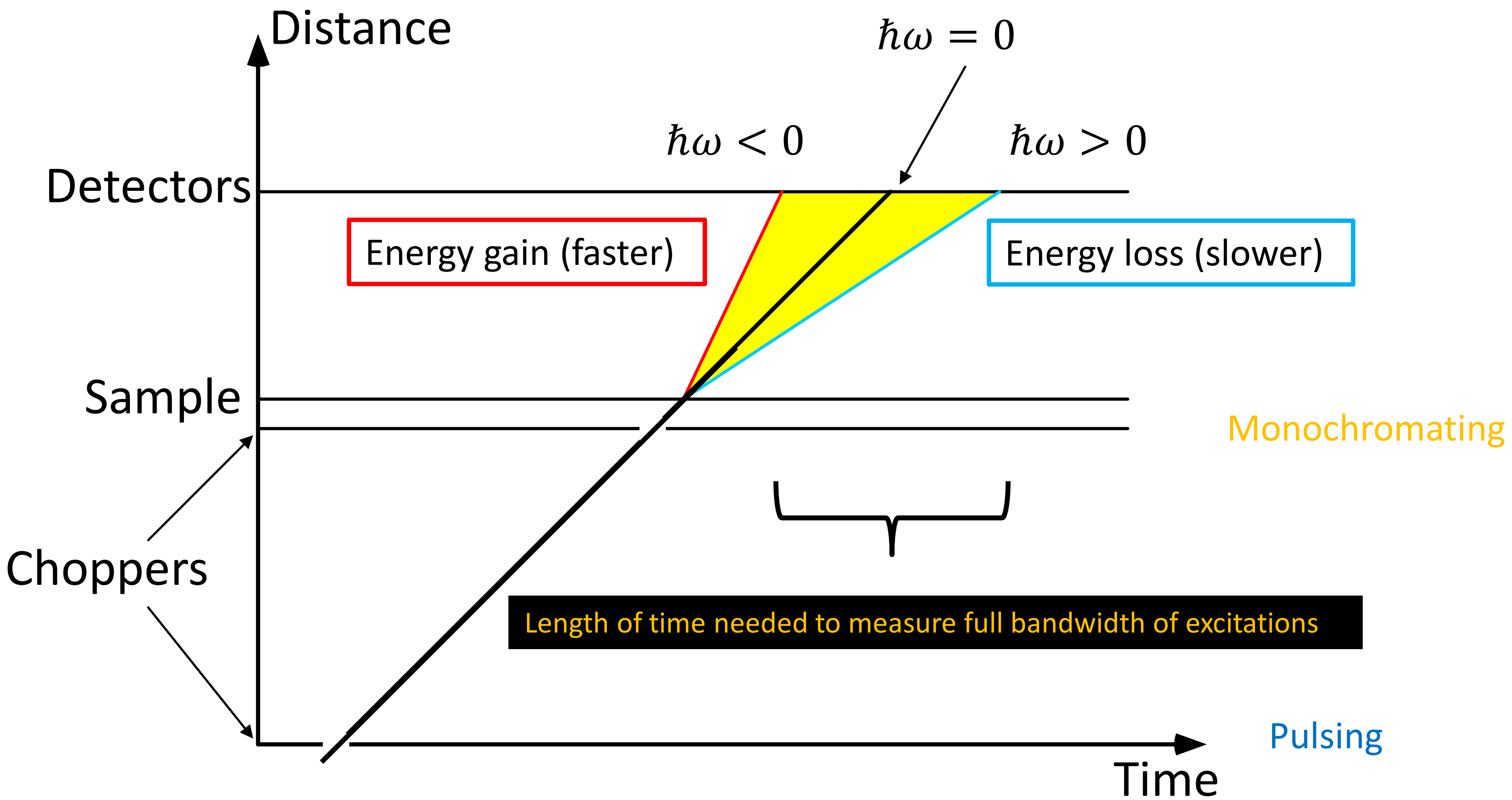


To double intensity and keep constant pulse time
Use two choppers and double the beam width

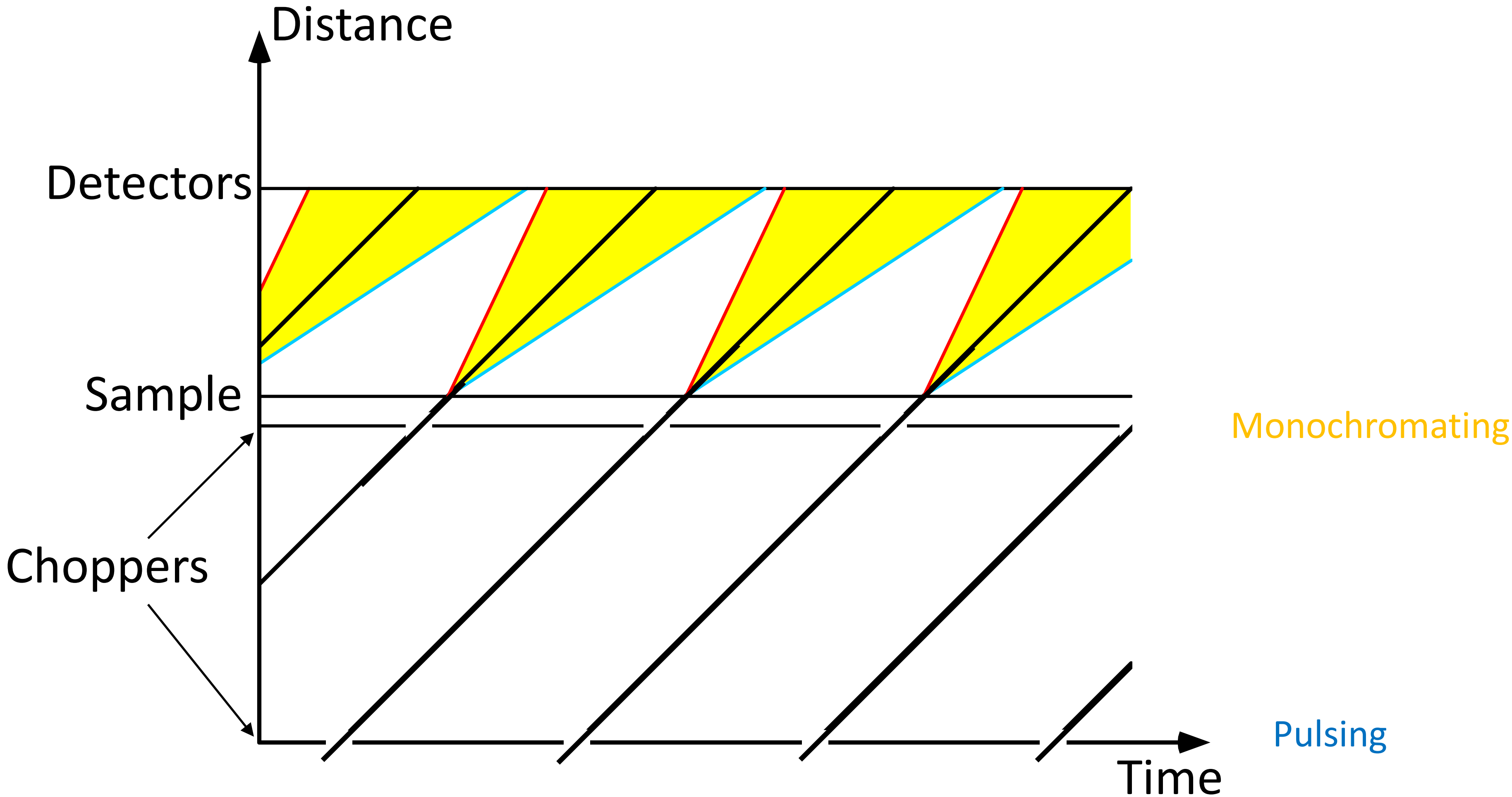
Why do we use more than 2 choppers?



Time-distance diagrams - single burst

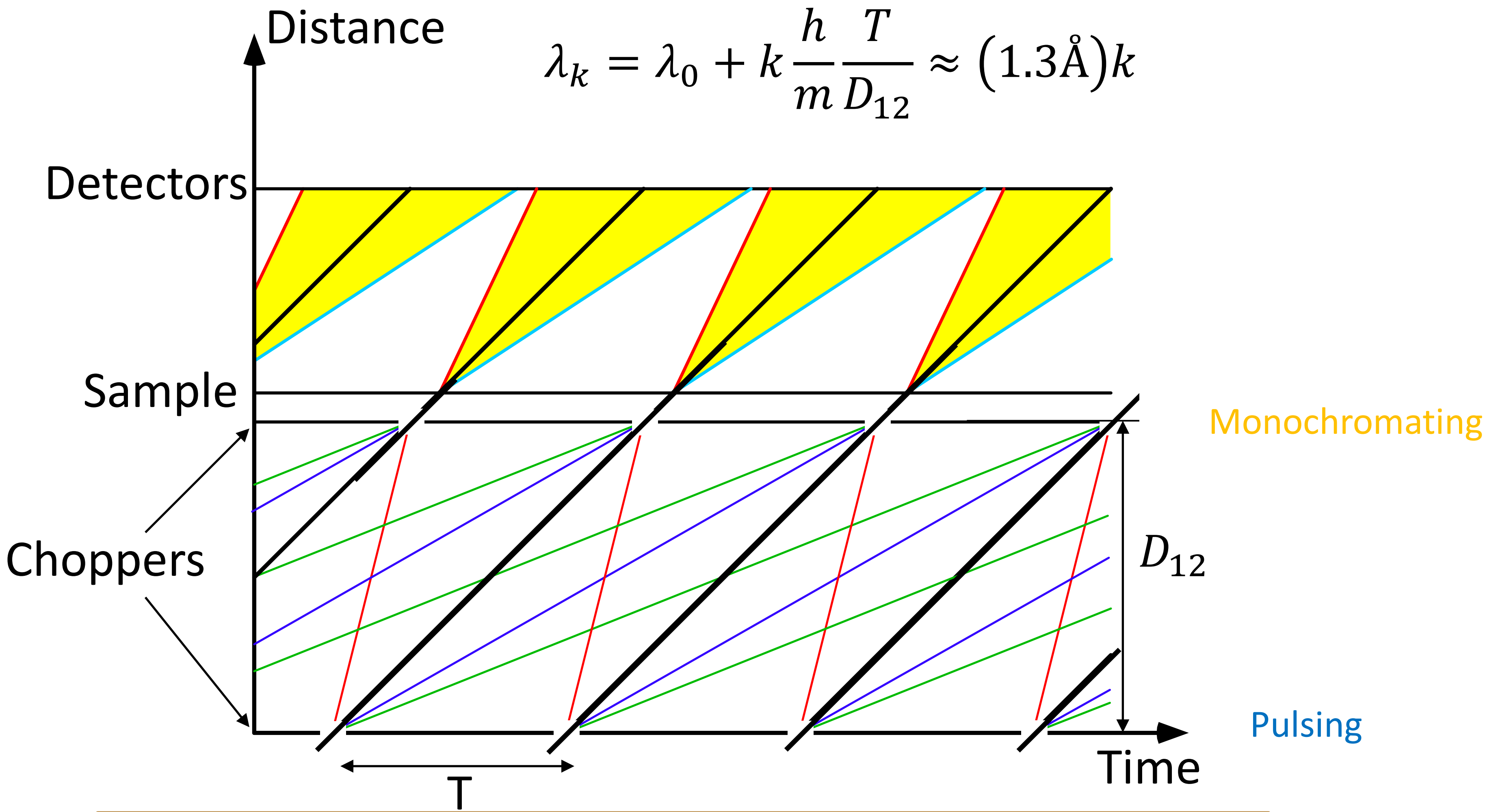


Time-distance diagrams - multiple bursts



Real experiment involves measuring this frame over and over and over and …

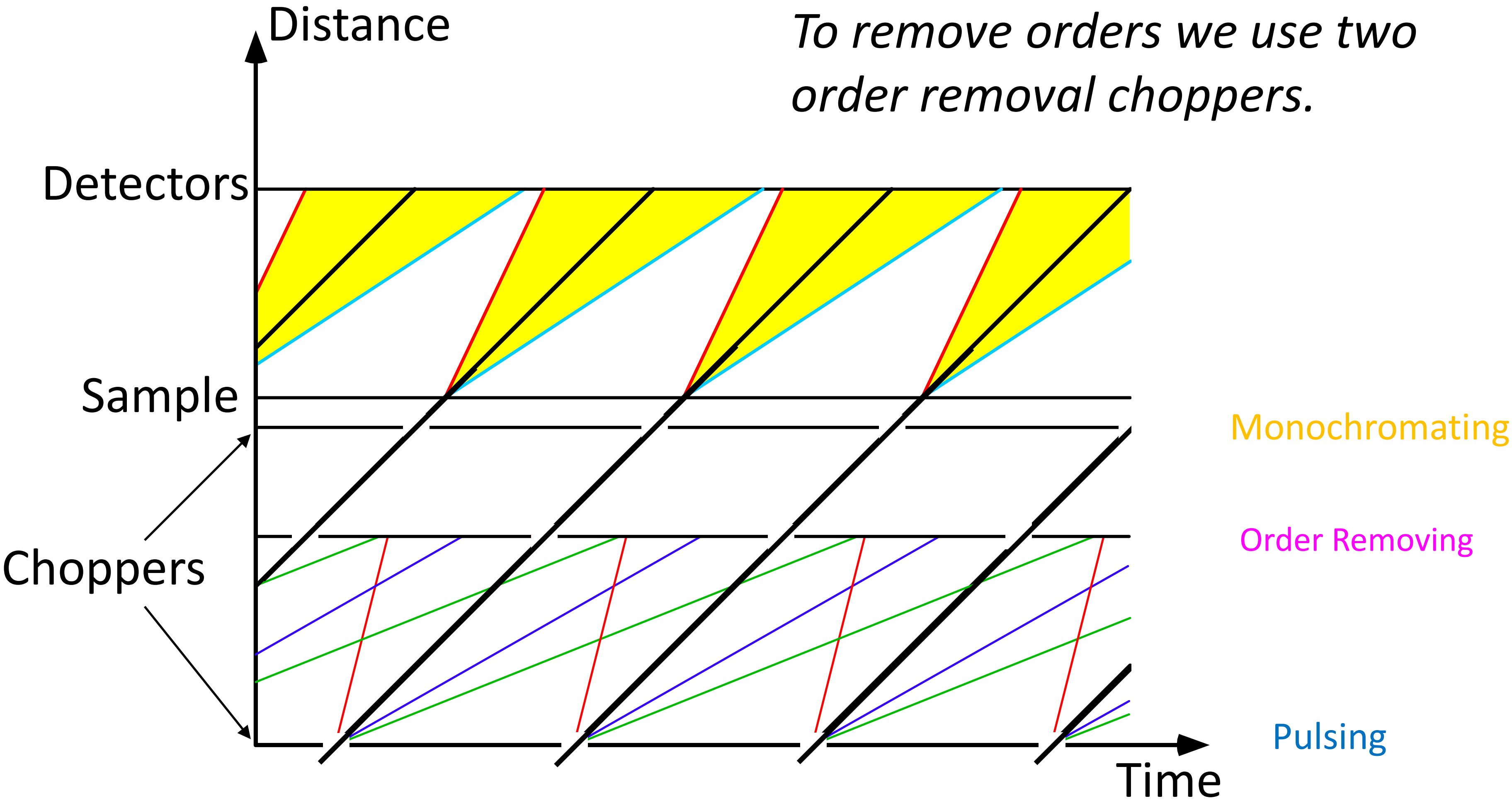
Complication 1: “contaminant” wavelengths



Faster or slower neutrons can also make it through the slots → multiple incident energies

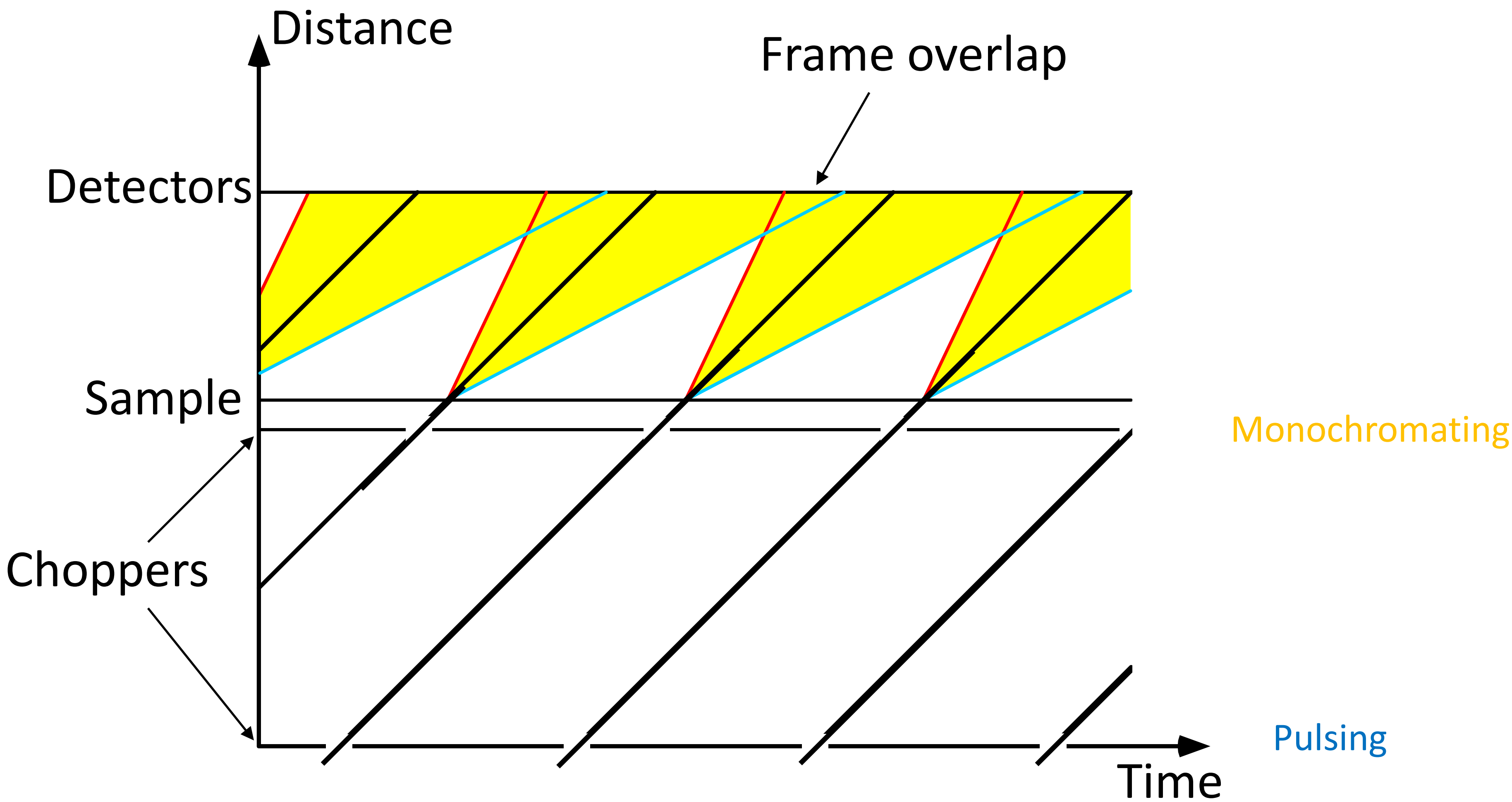
Solution 1: Removal of "contaminant" wavelengths

To remove orders we use two order removal choppers.



Faster or slower neutrons blocked by intermediate "order removing" choppers

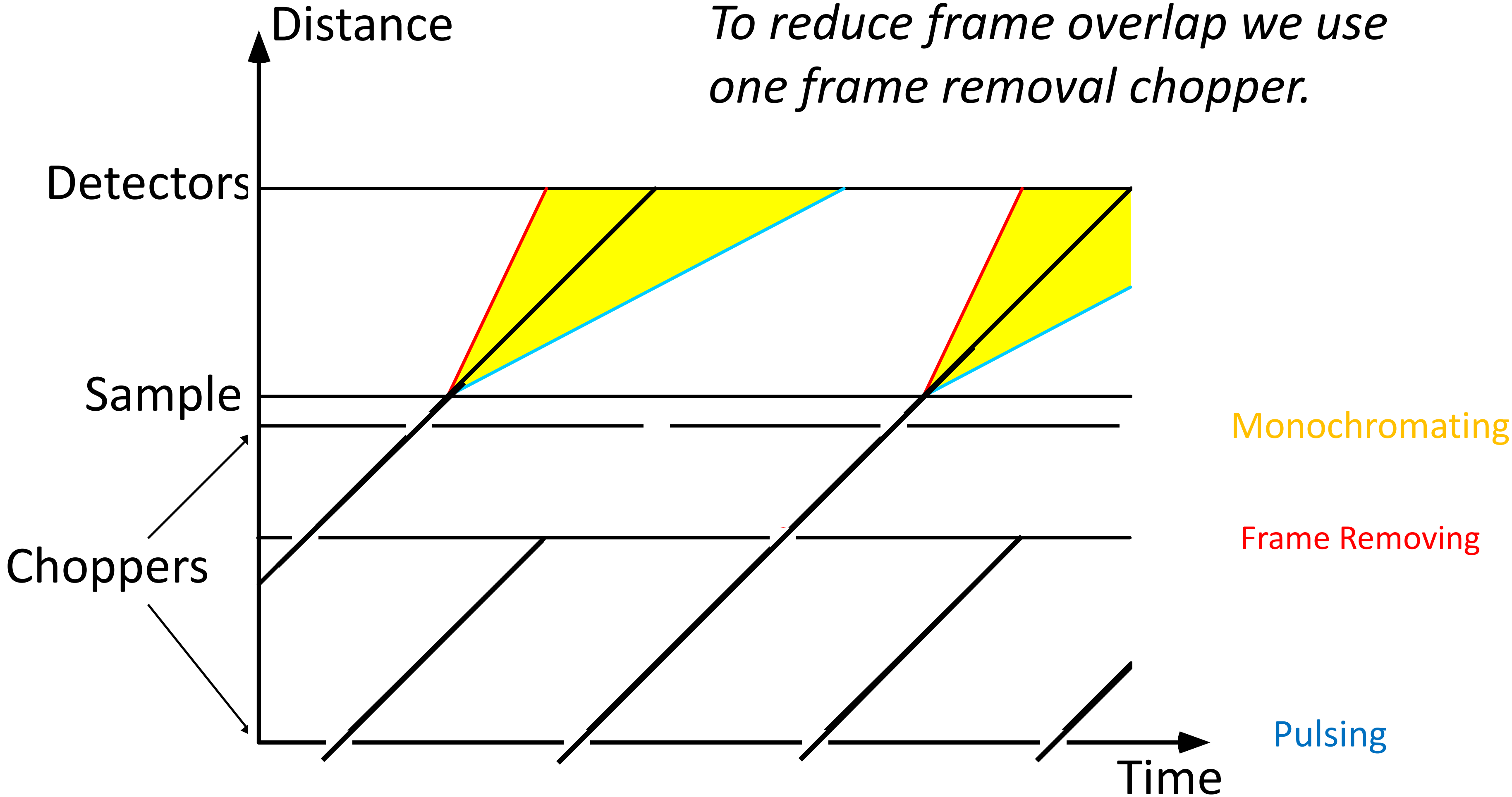
Problem 2: Frame overlap



Excitation bandwidth → time to measure longer than the pulse period

Solution 2: Removal of frame overlap

To reduce frame overlap we use one frame removal chopper.



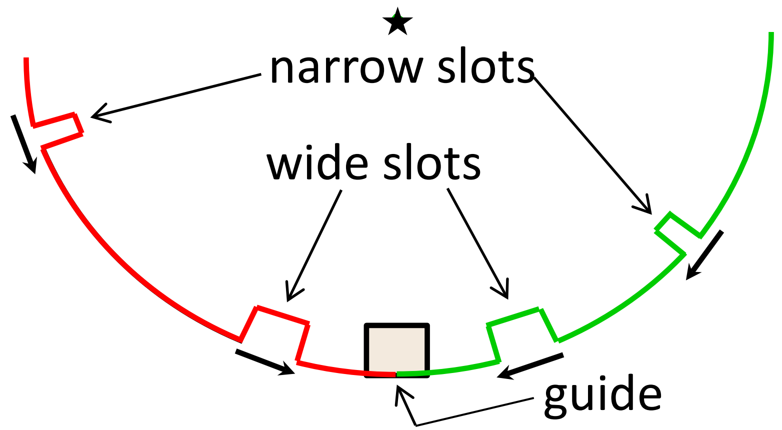
Literally, throw away adjacent pulses → reduce number of incident neutrons

The speed ratio denominator

1. Most choppers run with period T, frequency $f = 1/T$
2. Frame overlap removal chopper runs at lower speed:
   $f_S = f/m$ where m is an integer (m can equal 1)
   OR
   $f_S = f(m-1)/m$ where m is an integer greater than 1
   (needed because there is a minimum stable speed)
3. Either choice skips (m-1) pulses, e.g. m = 4 skips 3 pulses
4. The time between pulses at the sample is $T_S = mT$
5. m is called the "speed ratio denominator"

Multiple sets of slots / resolution modes

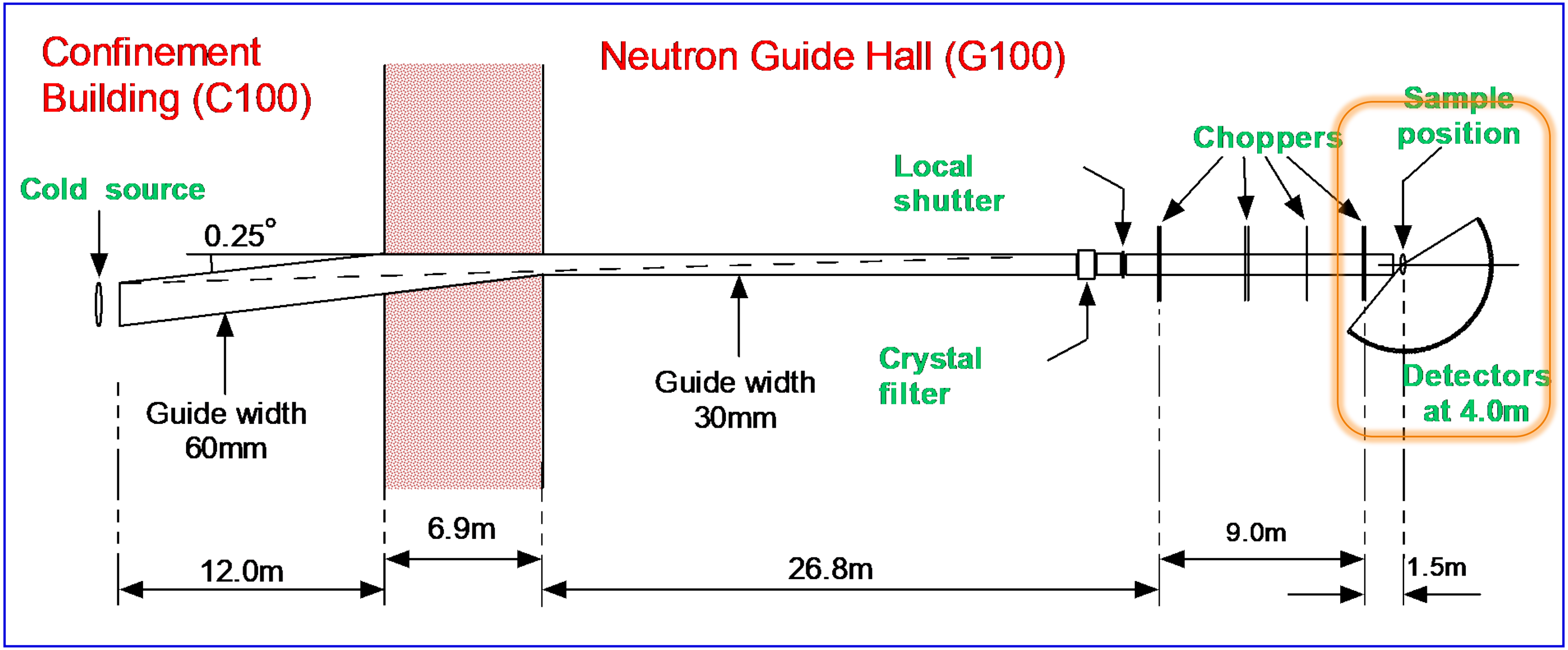
1. Slot width → time neutrons can pass through → length of the neutron pulse → energy resolution
2. DCS has 3 sets of slots
   1. Low, medium, high resolution (wide, medium, narrow)
   2. Only use one set at a time
3. Can select different energy resolution but maintain constant incident energy/wavelength, at cost of intensity



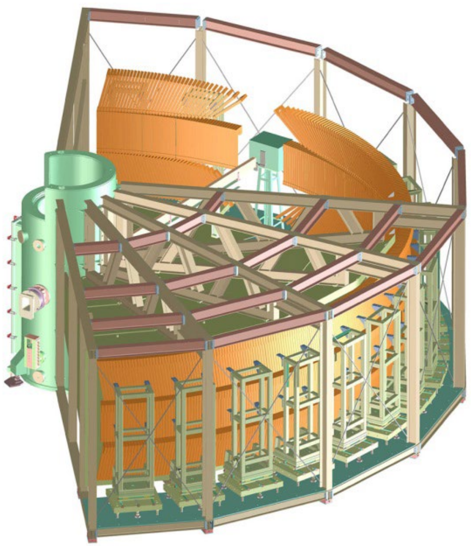
Slots are placed such that only "wide" will overlap in this configuration

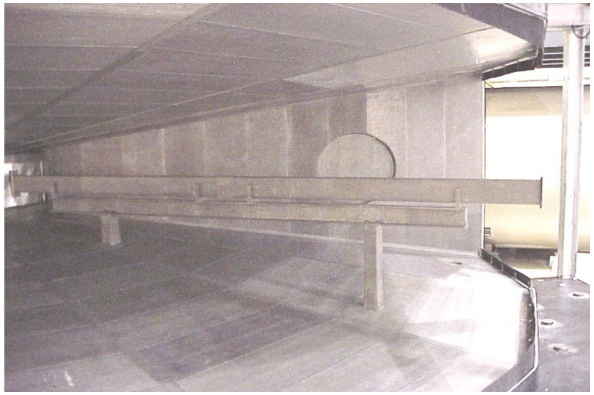
Detectors

DCS plan view



Flight chamber

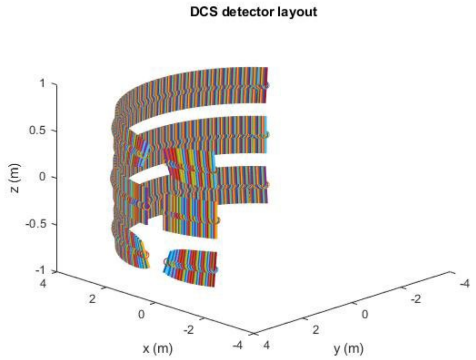




- Sample – detector distance 4 m
- Aluminum I-beam frame
  - Large welded sections bolted together
  - All inside surfaces clad with cadmium
- Argon balloon
  - Less scattering than air
  - Ultrathin (0.0075mm) Al window
  - It leaks, keep at + ~0.04 mTorr
- "Get lost" pipe to remove unscattered beam
  - Downstream beam monitor
  - Beamstop (polyethylene, cadmium, lead)
- 10-15 cm outside polyethylene shielding plus boraflex

Detectors

- 6 atm ^3He
- 913 detectors:
  - Large 2θ coverage
  - Middle bank: -30° to -5°, +5° to +140°
  - Upper, lower: -30° to -10°, +10° to +140°
- Arrangement
  - Identical 4 m sample distance
  - Sit on Debye-Scherrer cones



Data

DCS data structure – what we measure

Neutron scattering is a counting experiment

Detector events (counts/intensity) are stored in a 2-d histogram I(i,j)

i = 0…930 labels the ***detector*** (also beam monitor, etc)

Each detector sits at a known angle

j = 0…999 labels the ***time channel***

The time between pulses, T_S, is divided into N time channels of width $Dt=T_S/N$

This determines the time window of the measurement

At DCS, T_S is normally an integer multiple of 3000 μs and N=1000

Each coordinate (i,j) encodes ϕ (ie 2θ) and t_D

We want to calculate transferred momentum Q and energy ω

1. From I(ϕ,t) to the ddscs wrt time

Number of neutrons per second scattered at angle ϕ into solid angle dΩ, reaching detector within time interval $[t_D, t_D+dt]$

Number of atoms of sample in the beam

Solid angle subtended by detector

$$I(i,j) \Leftrightarrow I(\phi, t) = N\Phi \left[\frac{d^2\sigma}{d\Omega dt}\right] \Delta\Omega \Delta t$$

$$t = t_0 + j\Delta t$$

Width of time channel

Number of neutrons per second per unit area in the incident beam (incident flux)

Double differential scattering cross section (ddscs) wrt time; depends on ϕ and t

As $\Delta\Omega$ and Δt are constants, $\dfrac{d^2\sigma}{d\Omega dt} \propto I(\phi, t)$

2. From I(ϕ,t) to the ddscs wrt energy

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt} \cdot \frac{dt}{dE_f}$$

$$Since\ \ E_f = \frac{1}{2} m v_f^2 = \frac{1}{2} m \left(\frac{L_{SD}}{t_{SD}}\right)^2,$$

$$\frac{dE_f}{dt} \propto \frac{1}{t_{SD}^3},\ \ and\ \ \frac{dt}{dE_f} \propto t_{SD}^3,$$

$$Since\ \ \frac{d^2\sigma}{d\Omega dt} \propto I(\phi, t),\ \ \boxed{\frac{d^2\sigma}{d\Omega dE_f} \propto I(\phi, t) t_{SD}^3.}$$

Note: a signal constant in time is not constant in energy

3. From I(ϕ,t) to S(Q,ω)

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_S}{4\pi\hbar}\frac{k_f}{k_i}S(Q,\omega)$$

k_i is fixed and $k_f \propto \dfrac{1}{t_{SD}}$

$$Since \quad \frac{d^2\sigma}{d\Omega dE_f} \propto I(\phi,t)t_{SD}^3,$$

$$S(Q,\omega) \propto I(\phi,t) \cdot t_{SD}^4$$

S is typically the quantity that we use for further analysis

Samples

Powder and liquid samples

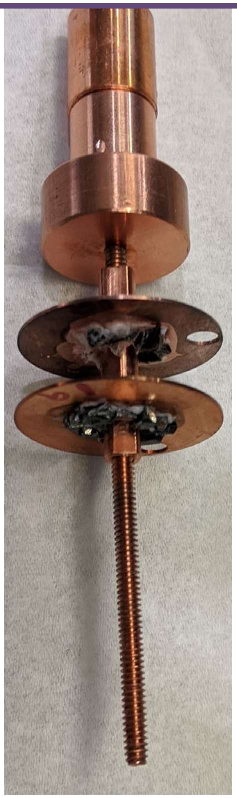
- Size
  - Low-res beam is 10cm tall x 3cm wide
  - Tall and skinny cans for powder/liquid
  - More sample is generally better, typically gram masses
- Shape
  - Empty cylinders for maximum volume
  - Annular cans for strong scatterers (hydrogen)

Cylindrical can

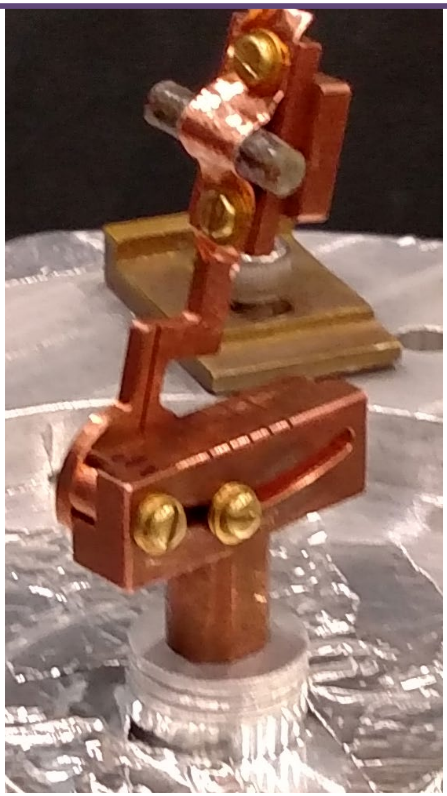
Annular can

Single crystals

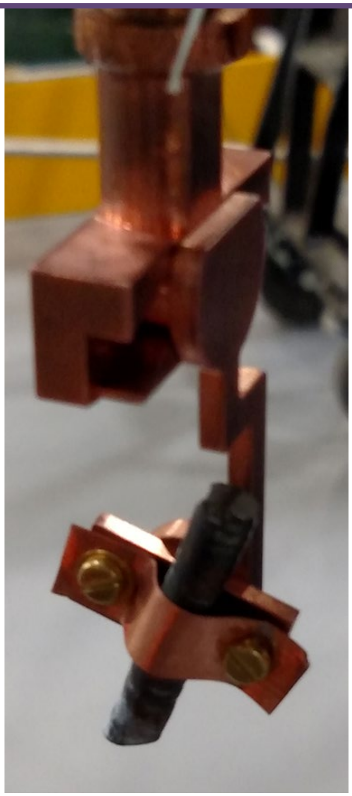
Coaligned small crystals



Gram-sized crystal on goniometer



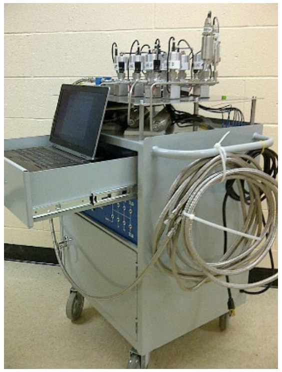
Fridge-mounted goniometer

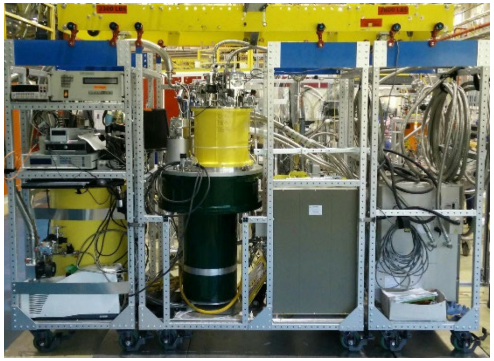


Due to size, shape, and orientation variations and requirements, holders are varied and often custom-made

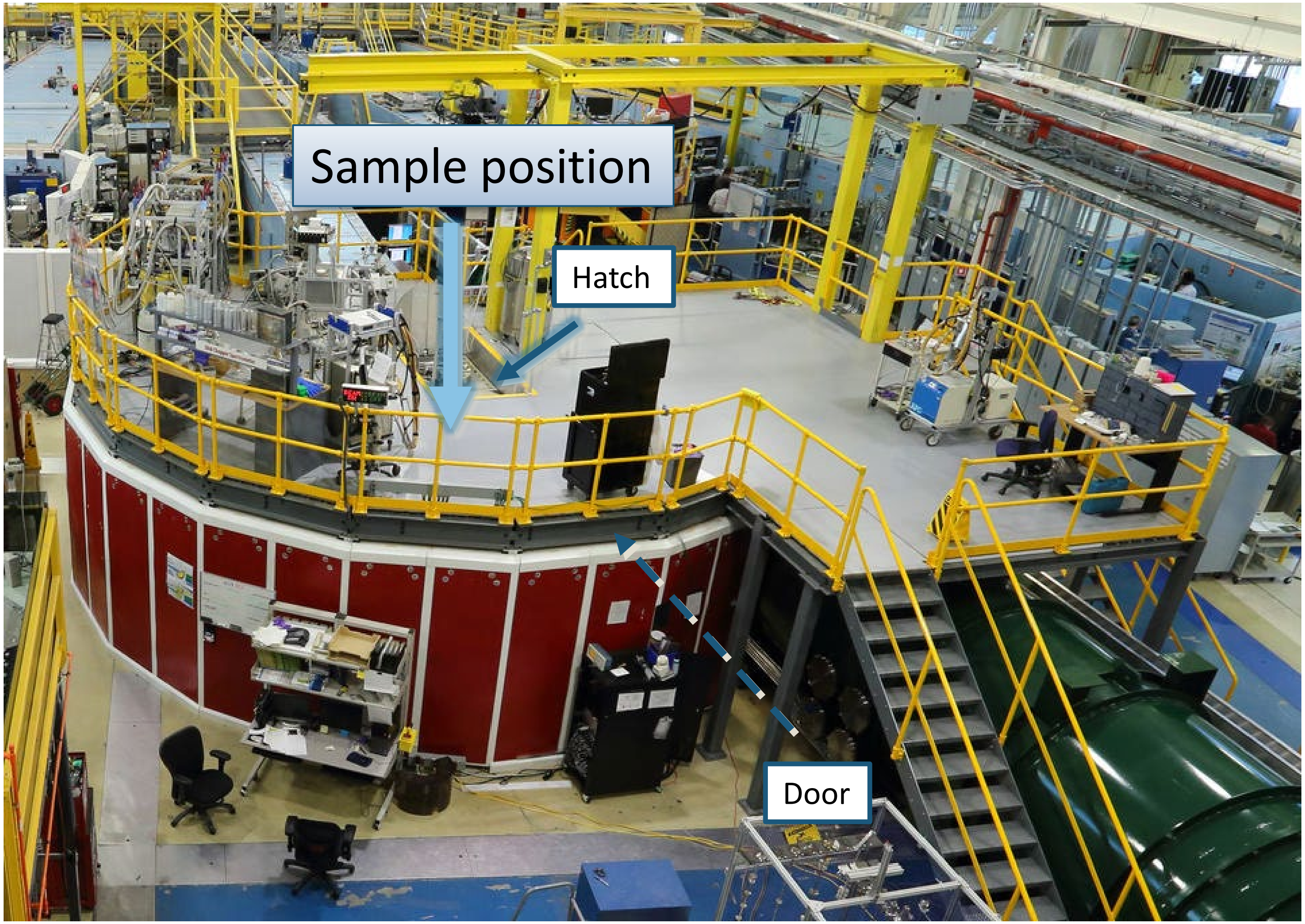
Sample environment

- Temperature
  - Cryostats (cold, heat)
  - Millikelvin fridges
  - Furnaces (high heat)
- High pressure
- Gas loading
- Magnets
- *Can be the most complicated part of experiment*





DCS looking toward reactor

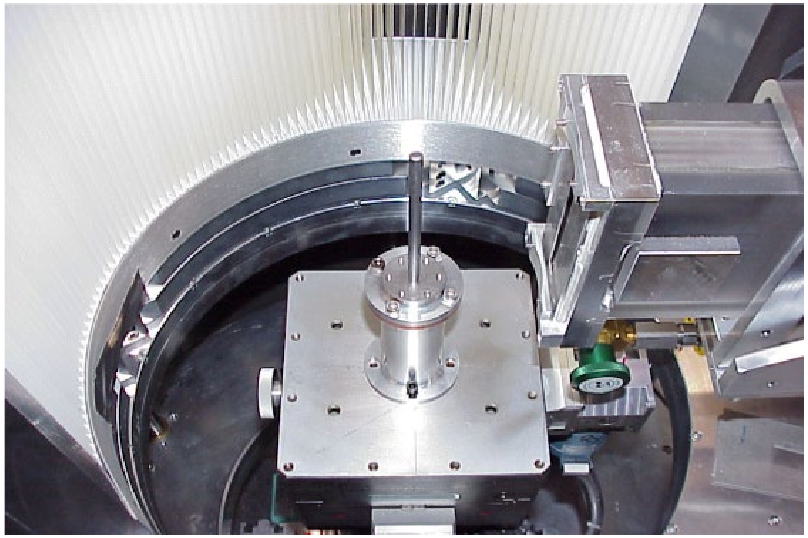


Sample chamber

- ID = 864 mm
- Access from above (hatch) and side (door)
- Sample stage
  - Holds sample environment
  - XYZ motors
  - Rotation
- Radial collimator:
  - Points at sample position
  - ID 400mm, OD 600mm,
  - Blade separation 2°, blade height 250mm, spans 170°
  - Oscillated through 2°

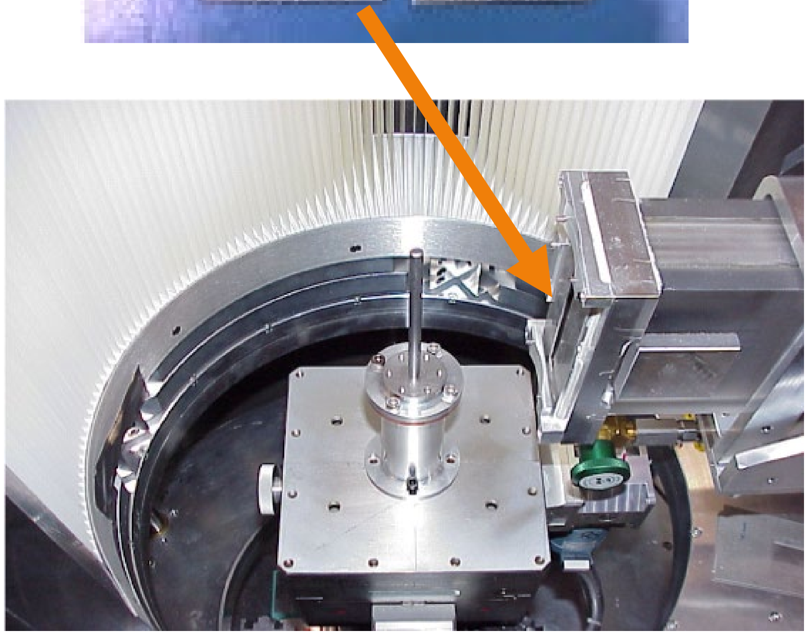
Hatch

Door



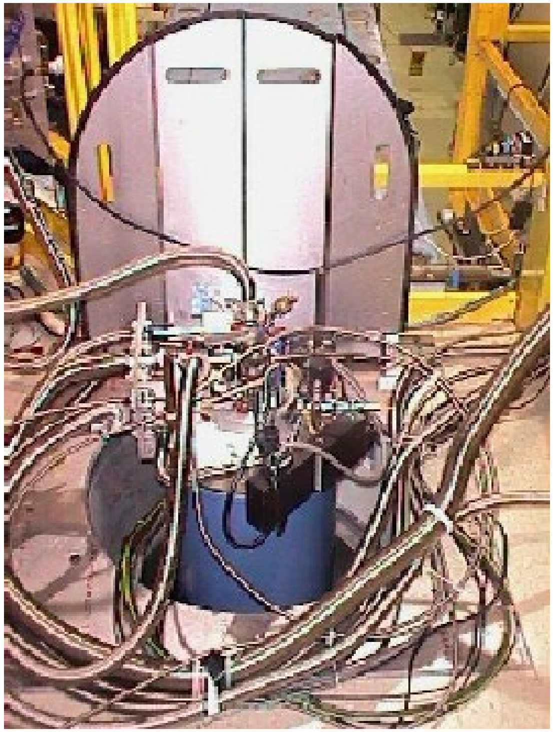
Looking down at sample stage from doorway

Beam masks



- Samples don't always fill beam
- Cadmium masks block cold neutrons
  - Make beam shorter, narrower
  - Reduce scattering off of cans and holders
  - Choose width, height
  - Throwing away neutrons
- Place at end of guide

Ready to go



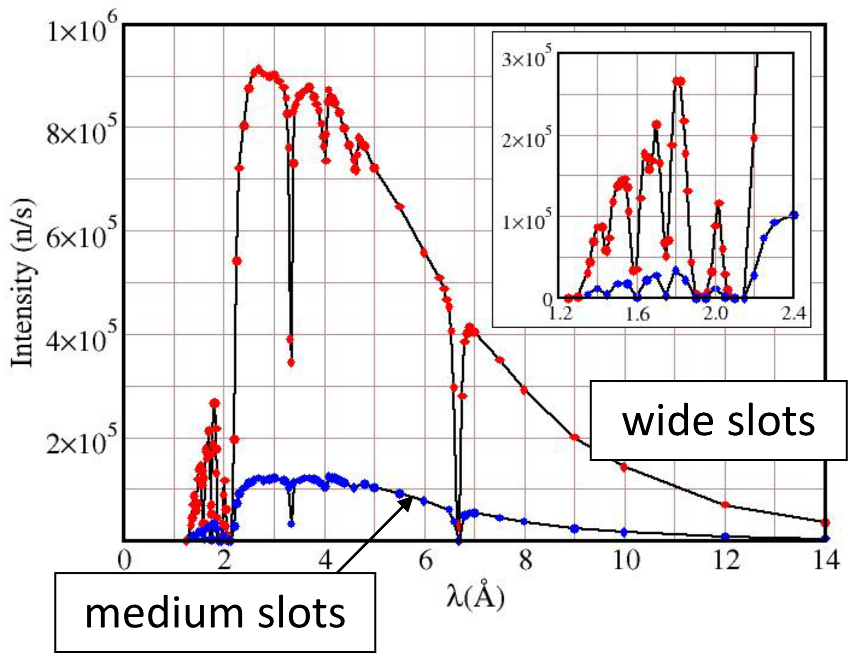
In addition, need to manage vacuum pumps, gas pressure, cryogen levels, etc.

Cryostat in the pit, with wires and plumbing laid out
Even more complicated – rotation (cable management)

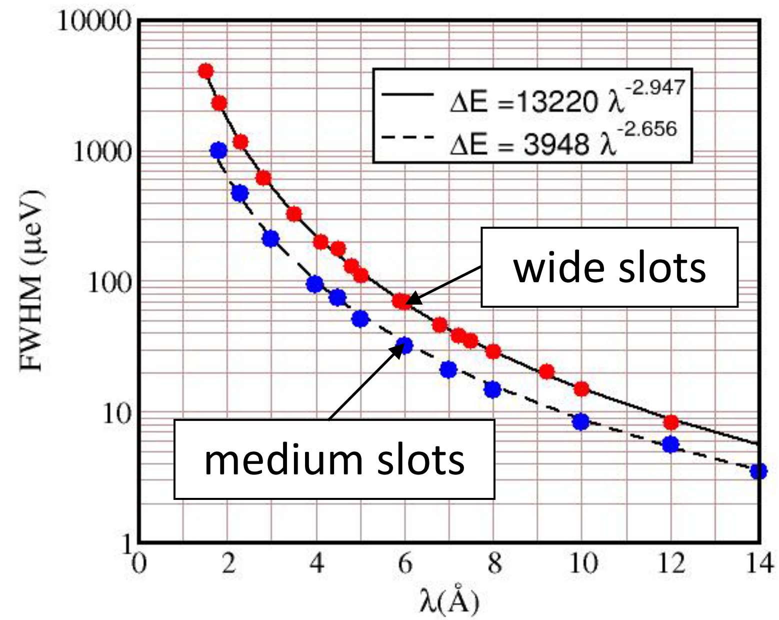
Planning the measurement

Choice of incident wavelength/energy

Intensity at sample I(E)



Resolution width ΔE

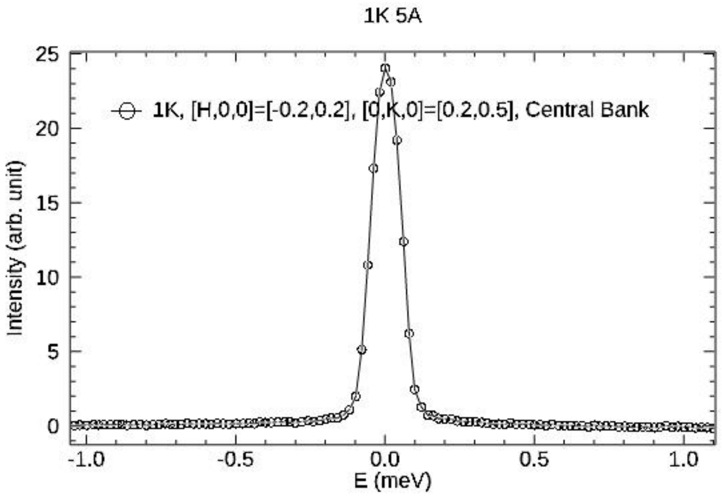


- Highest intensity around 2.5−4.5Å
- At long λ, I(E) drops ≈ 50% for every 2Å
- Energy resolution width ΔE varies roughly as $1/\lambda^3$
- Q range and Q resolution ∝ 1/
- λSharp dips due to graphite filter Bragg peaks

$E_i = 81.8 / \lambda^2$

What is resolution?

- How precisely DCS determines E and Q
  - Defined by instrument design
  - Depends on chopper settings
    - Wavelength / incident energy
    - Pulse duration / slot width-rpm
- Energy: broadening of the true energy transfer
- The instrument resolution can change the apparent lineshape of excitations, e.g. quasielastic
- Momentum: determined by (fixed) detector density and solid angle



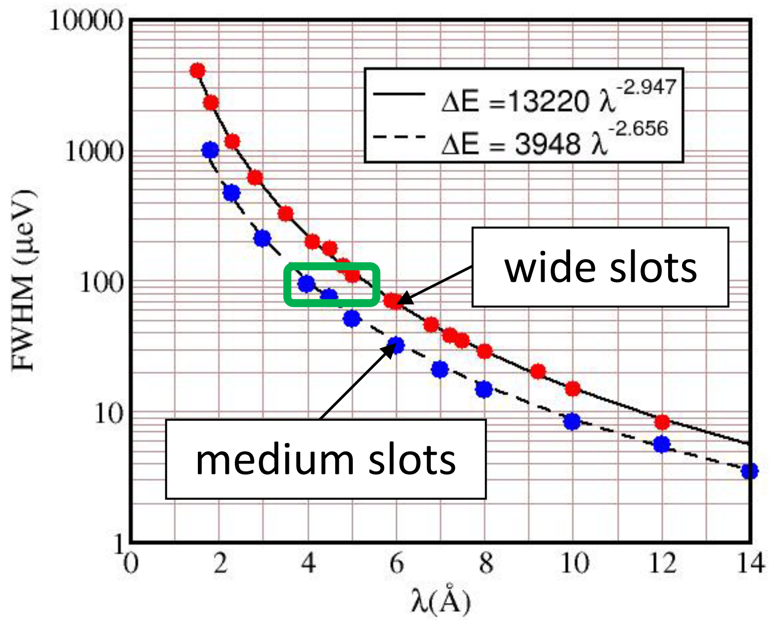
Elastic scattering should be a delta function, but is broadened by the finite pulse width (making pulses shorter lowers the intensity)

Which settings to choose?

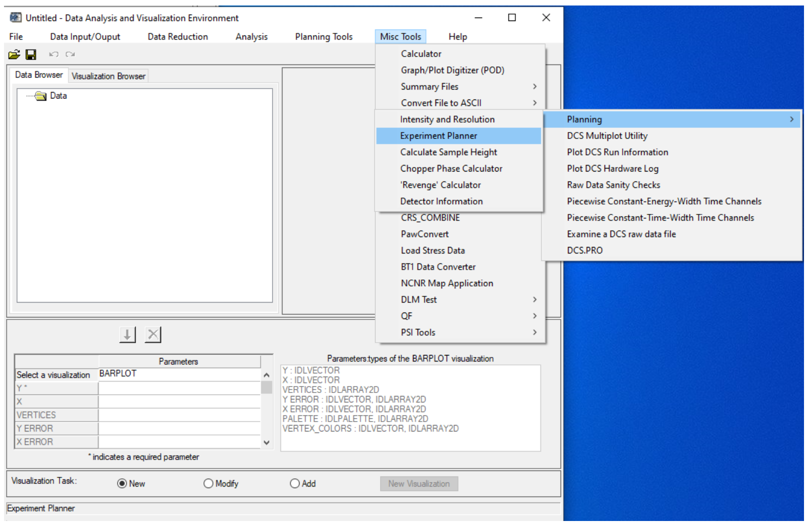
For example, say you expect that you need E resolution of 100 μeV
Choose 5A on low resolution (wide slots) or perhaps 4A on medium resolution?

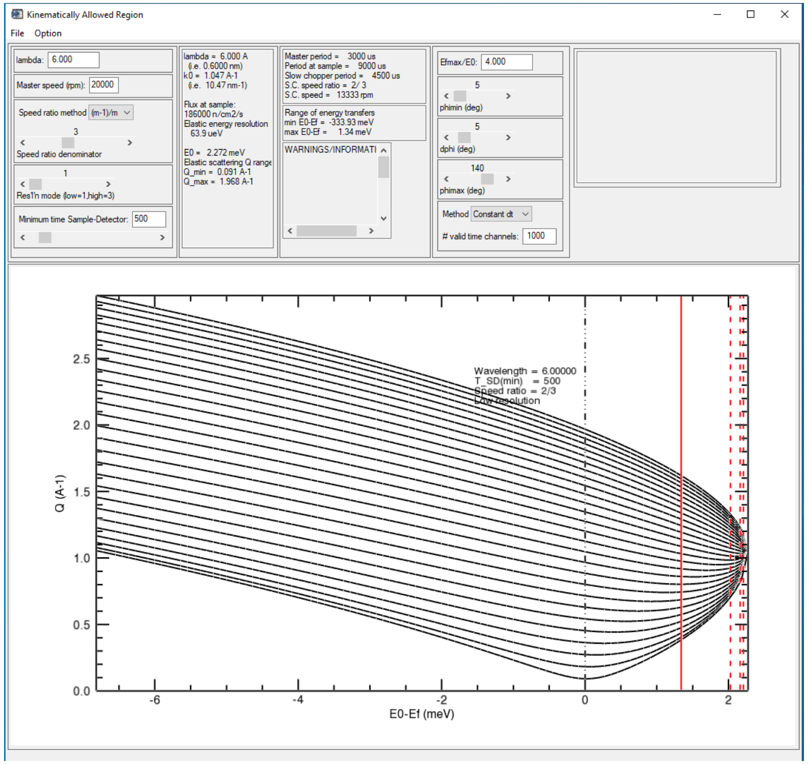
1. Wavelength (incident energy)
   – Constrains Q and E range
   – Defines resolution
2. Speed ratio / frame overlap
3. "T_{SD}(min)" time-of-flight from sample to detector

Resolution width ΔE



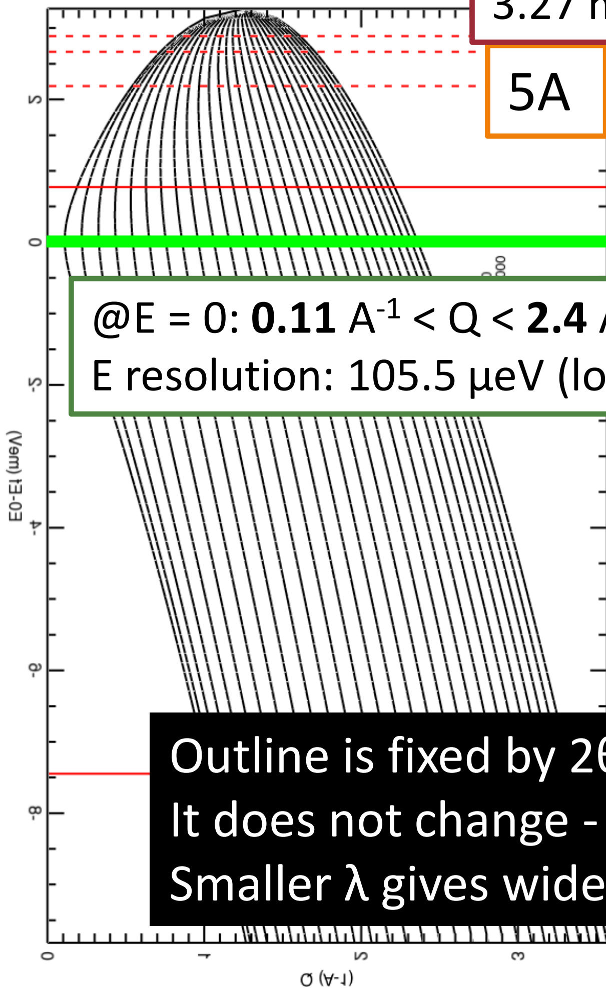
Simulating the DCS experiment





https://www.nist.gov/ncnr/dave-data-analysis-software

Compare 5A and 4A: E, Q range



3.27 meV

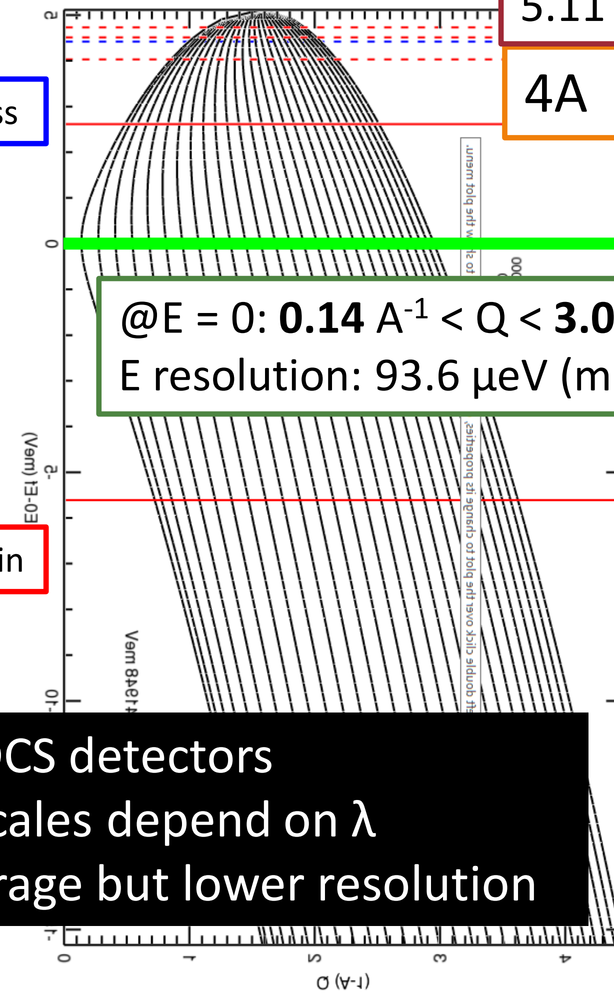
5A

@E = 0: **0.11** A^{-1} < Q < **2.4** A^{-1}
E resolution: 105.5 μeV (low)

Neutron energy loss

E = 0

Neutron energy gain



5.11 meV

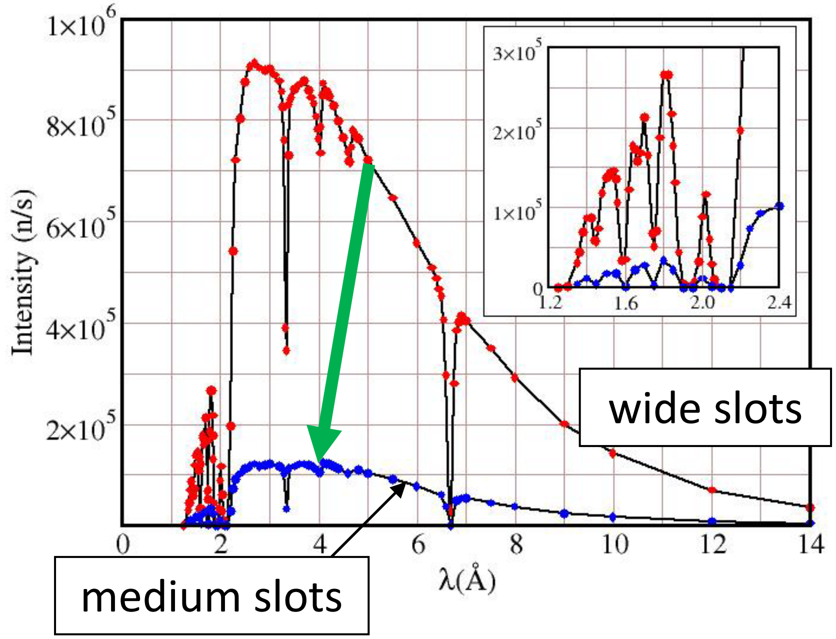
4A

@E = 0: **0.14** A^{-1} < Q < **3.0** A^{-1}
E resolution: 93.6 μeV (medium)

Outline is fixed by 2θ coverage of DCS detectors
It does not change - only the axis scales depend on λ
Smaller λ gives wider Q and E coverage but lower resolution

Why not always use medium resolution?

Intensity at sample I(E)



Medium resolution has 7x fewer neutrons
High resolution is almost never used

Which settings to choose?

For example, say you expect that you need E resolution of 100 μeV
Choose 5A on low resolution (wide slots) or perhaps 4A on medium resolution?

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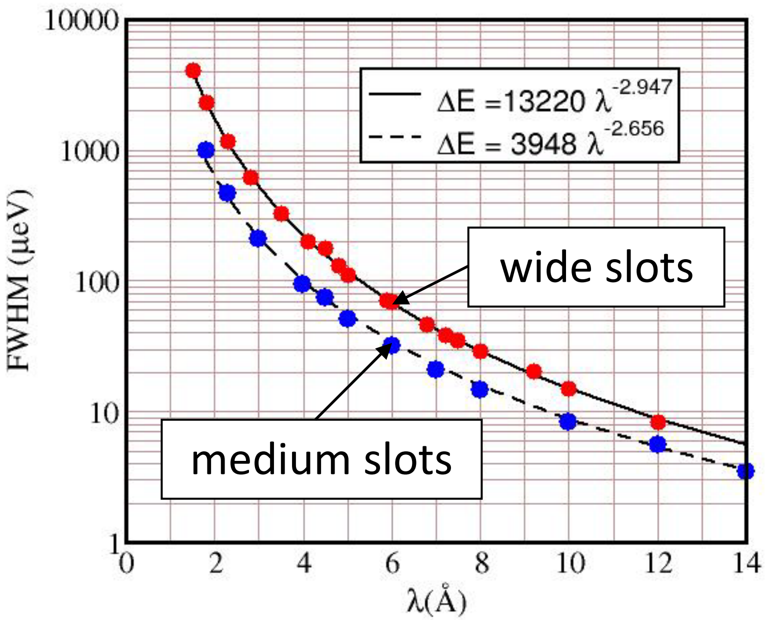
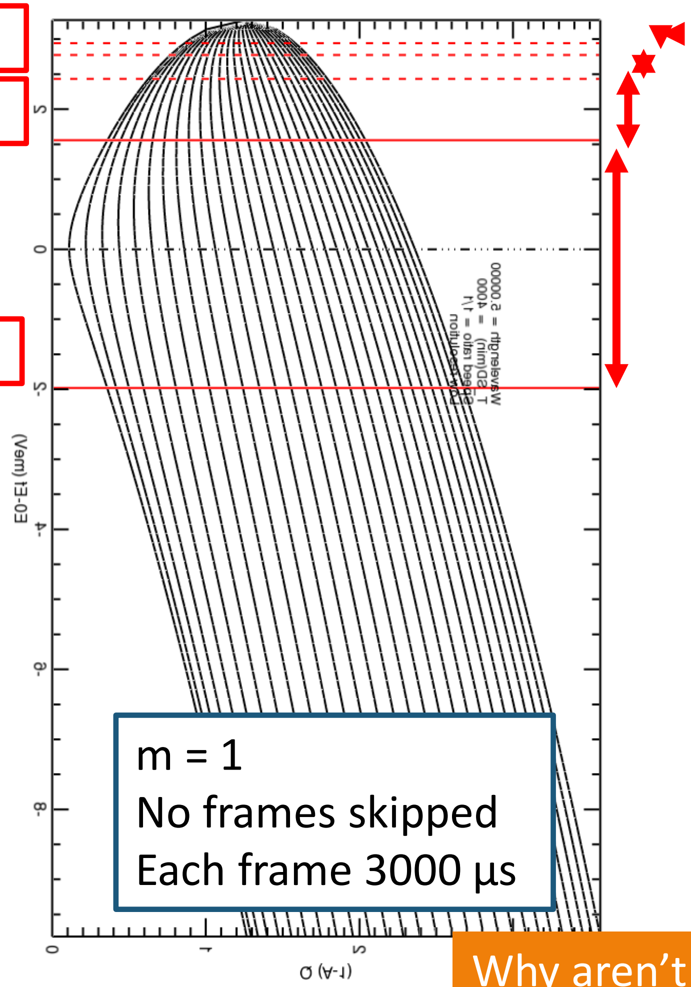
   - Constrains Q and E range
   - Defines resolution
2. Speed ratio / frame overlap
3. "T_{SD}(min)" time-of-flight from sample to detector

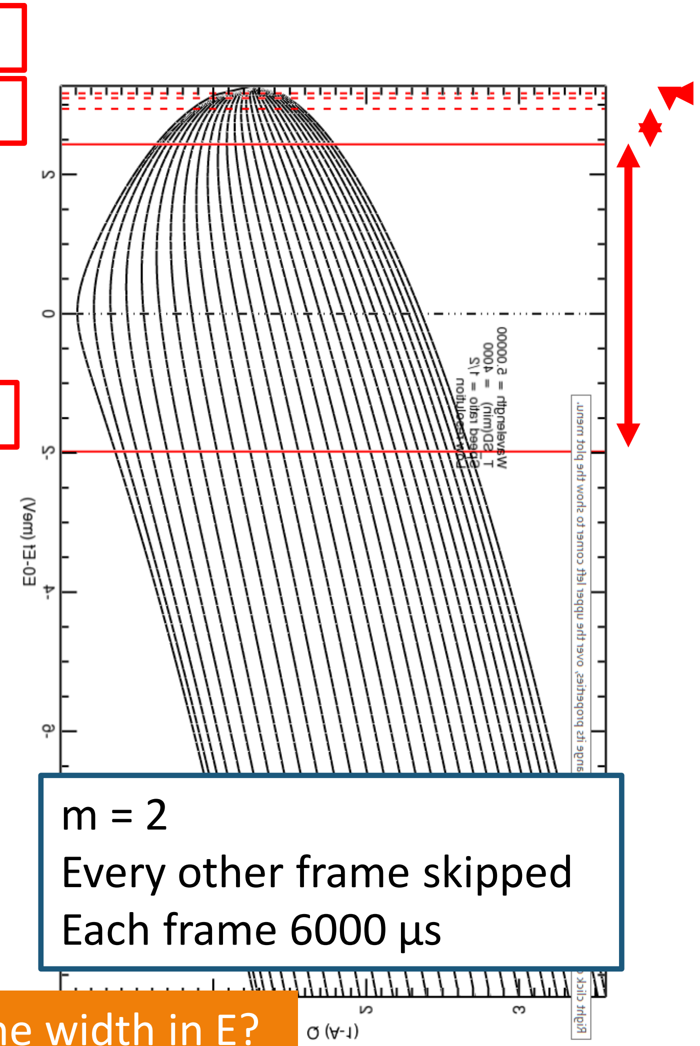
Resolution width ΔE



Frame timing and m



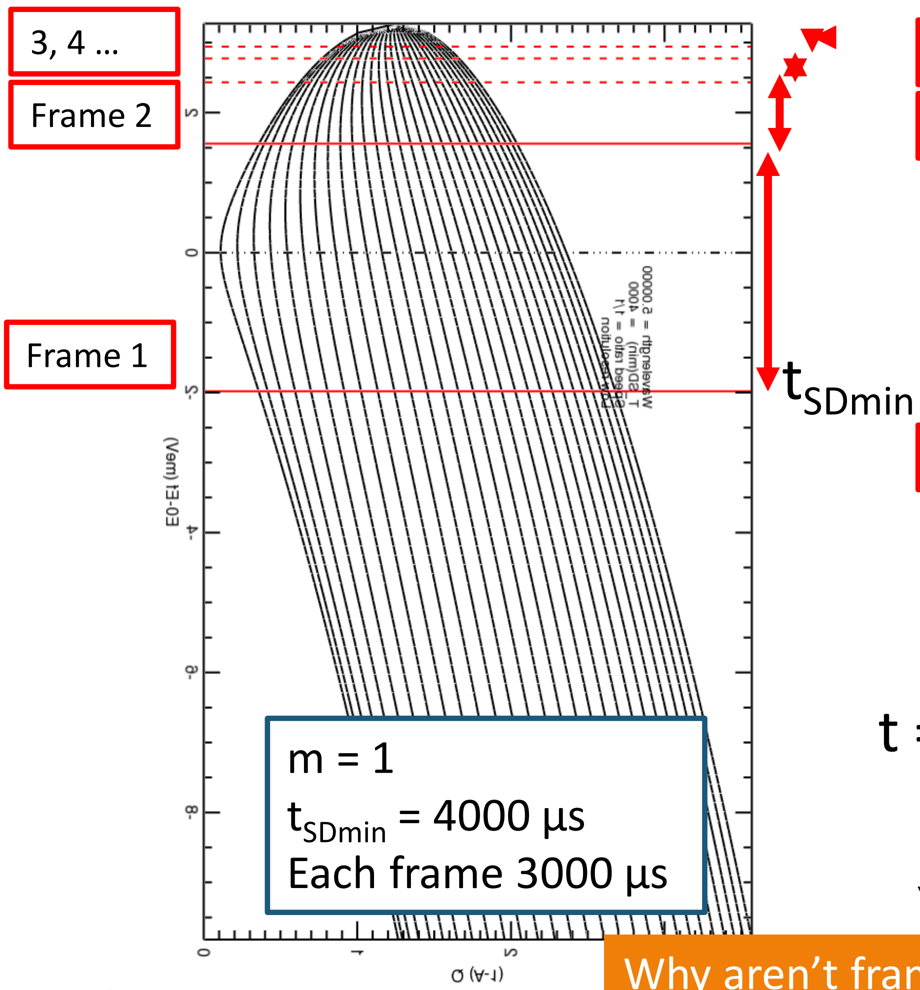
m = 1
No frames skipped
Each frame 3000 μs

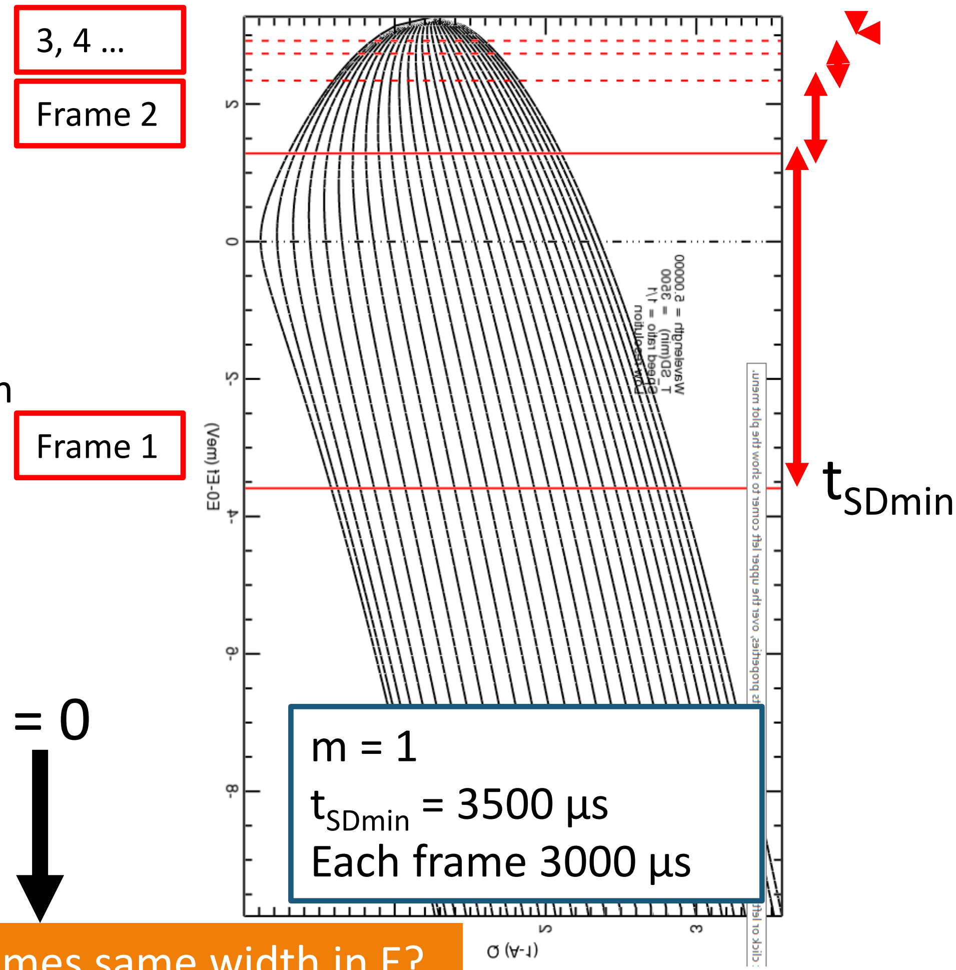


m = 2
Every other frame skipped
Each frame 6000 μs

Why aren't frames same width in E?

Frame timing and t_{SDmin}



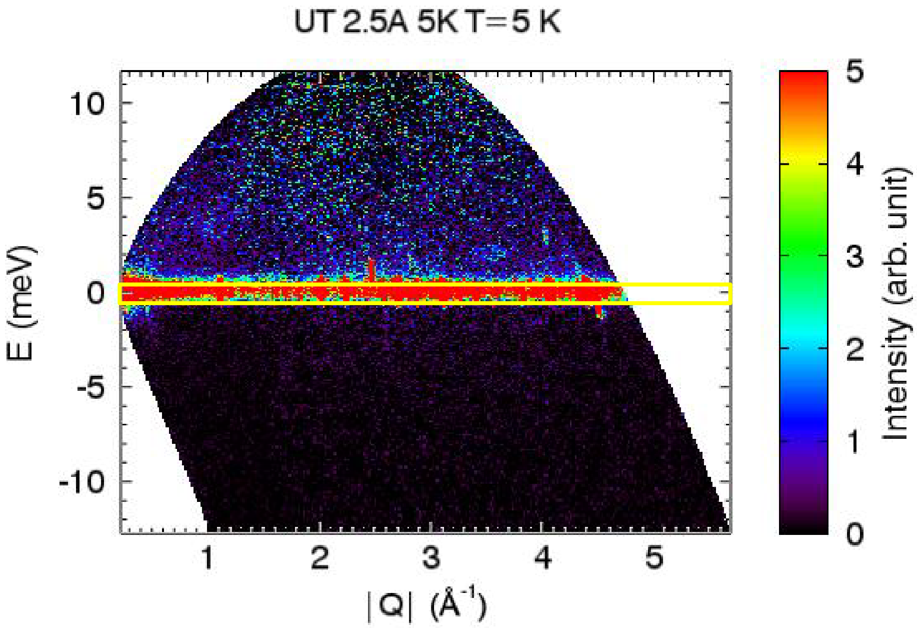


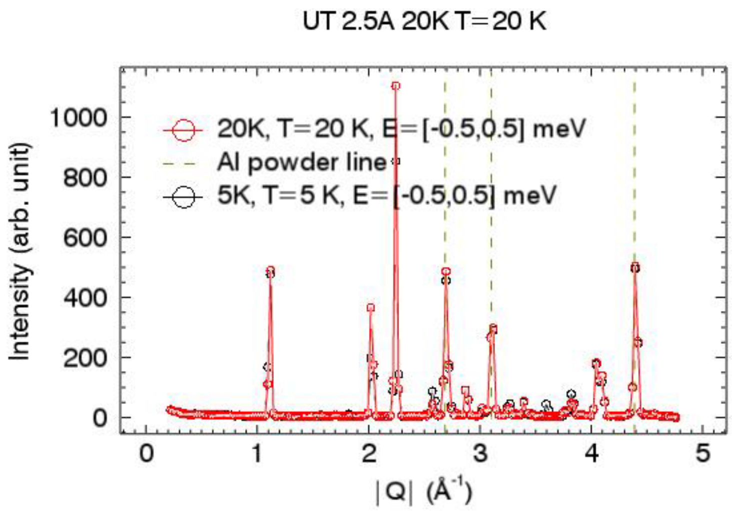
t = 0

Why aren’t frames same width in E?

What DCS data look like

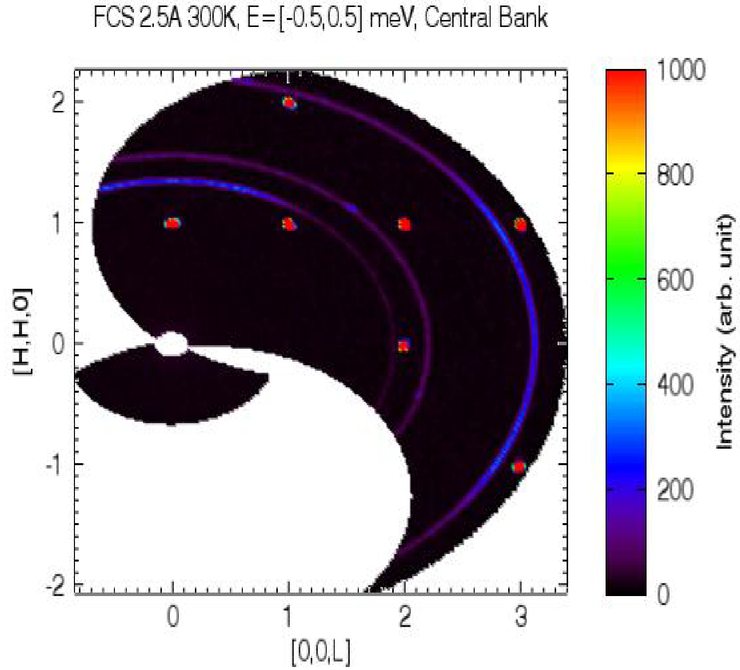
Powder diffraction on DCS





Diffraction is elastic ($\Delta E = 0$) scattering, analogous to x-ray diffraction

Single crystal diffraction



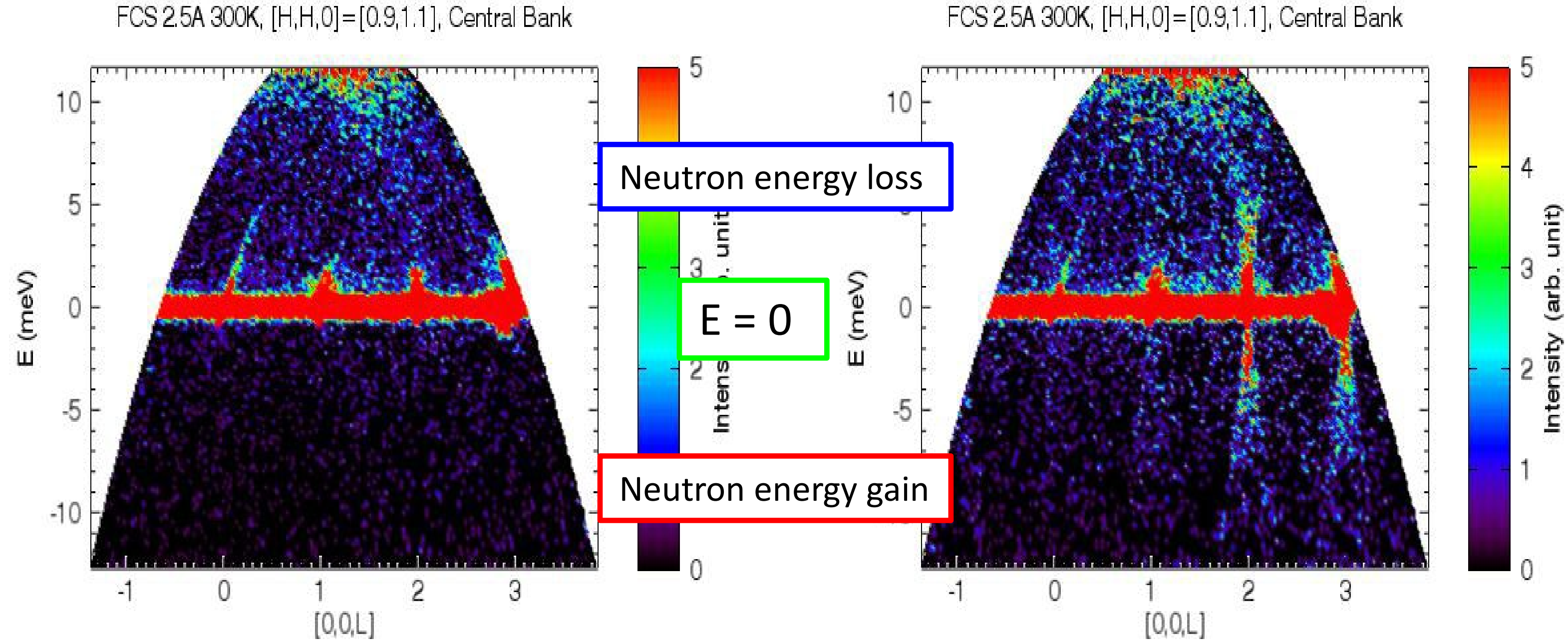
- Rotate crystal to collect
- This is E = 0
- Bragg peaks from crystal
- Powder rings from sample holder and cryostat

Effect of temperature on excitations

Phonons in a single crystal

17.5 K

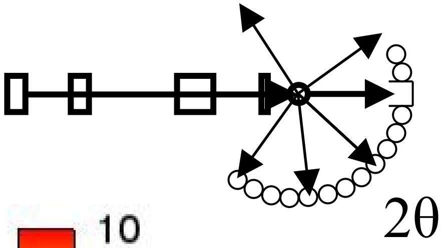
300 K

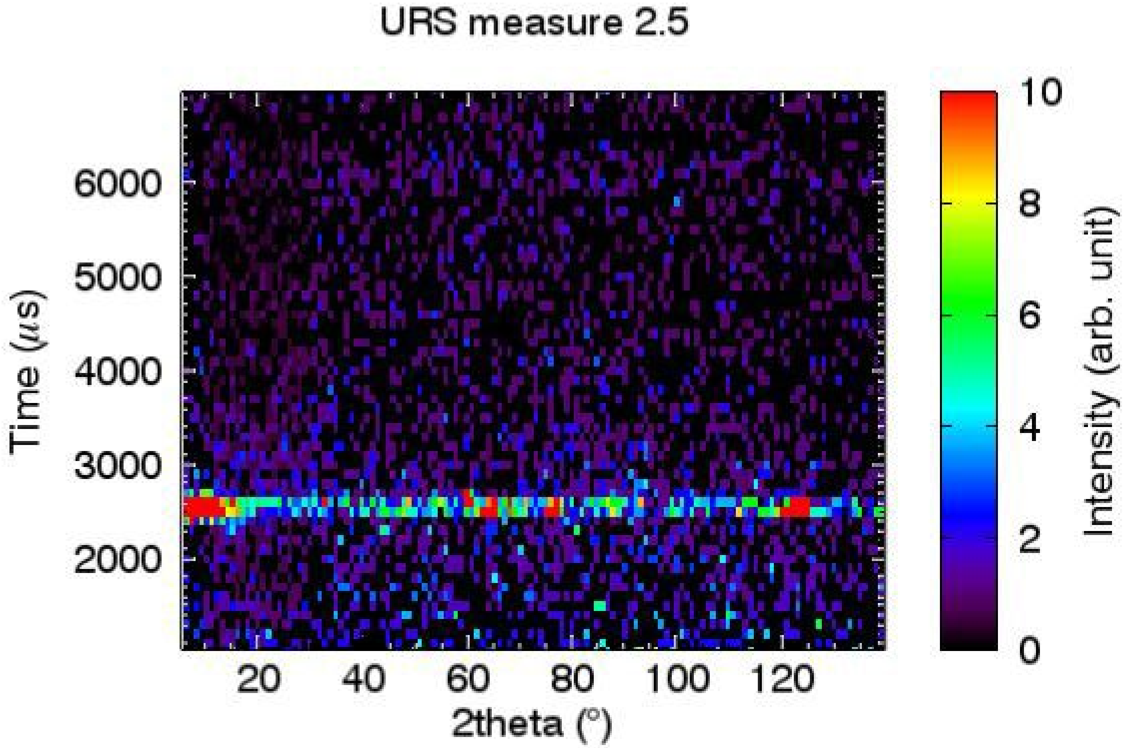


Low T – no thermal excitations in sample to excite neutrons

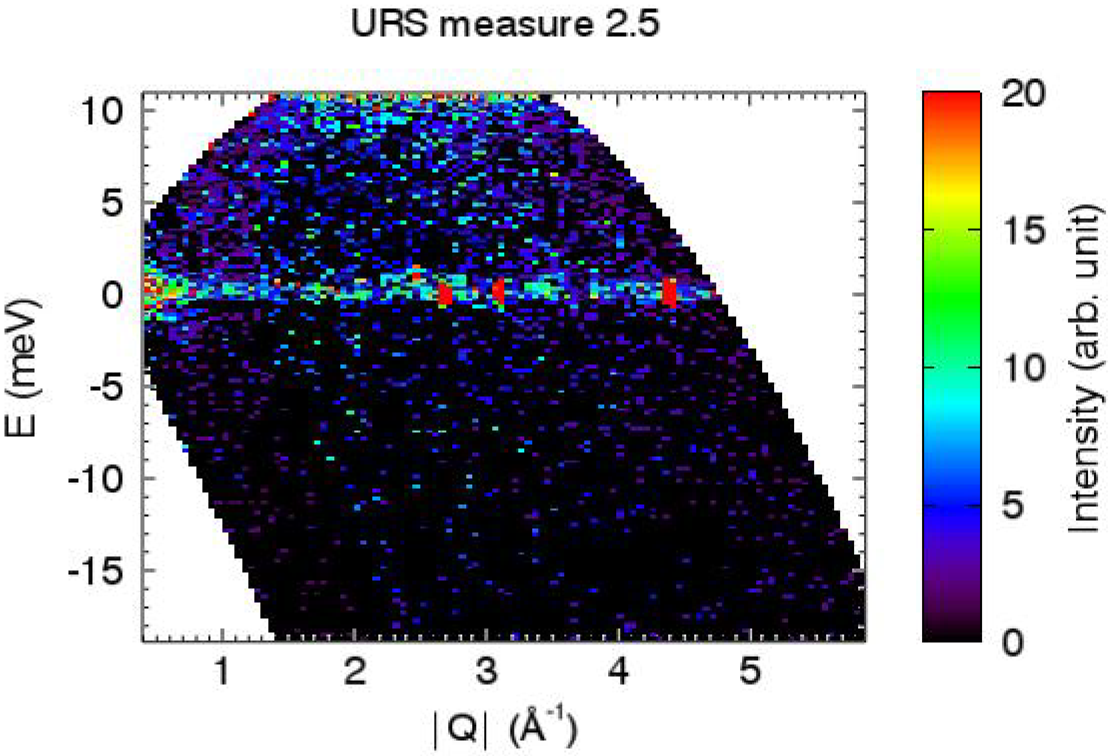
High T – sample excitations thermally populated, can transfer energy to neutrons

URu_2Si_2: measure I(2θ,t)



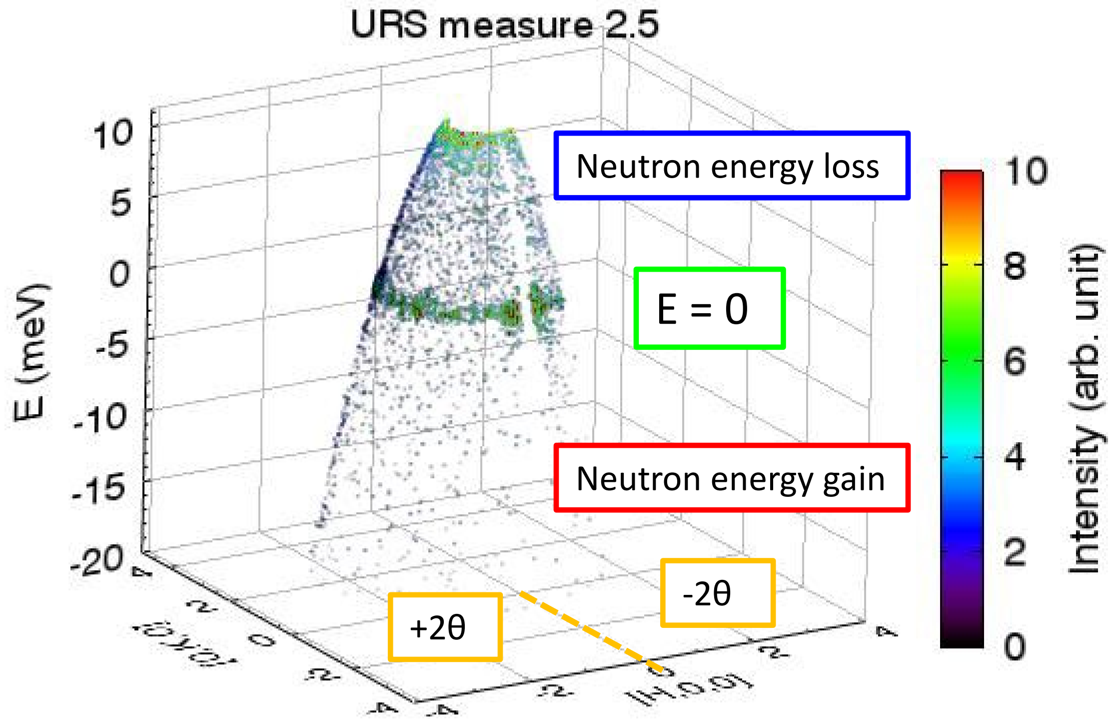


URu_2Si_2: I(2θ,t) → S(Q,ω)



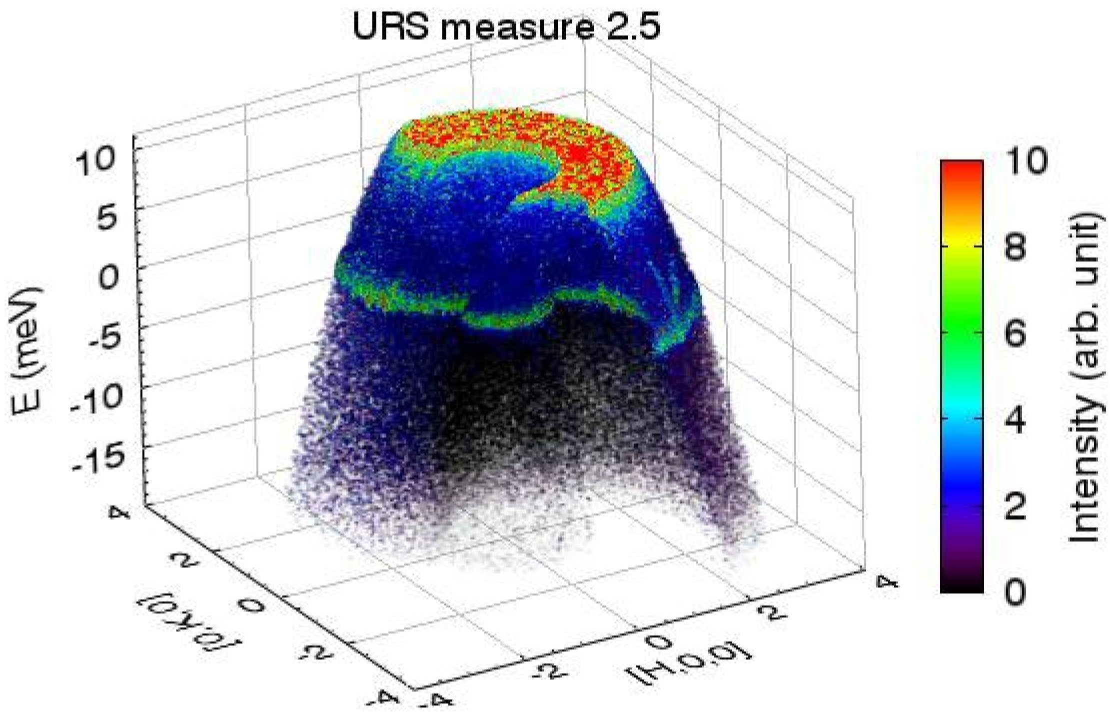
URu_2Si_2: $S(Q,\omega)$ is 3D b/c Q is a 2D vector

OK, Q is really 3D but we only measure in the horizontal plane on DCS
The shape below is the same as on the previous slide, but now includes direction



This is important for single crystals, but not powders and liquids

URu_2Si_2: Rotating the crystal fills in the Q,E volume



Rotating the crystal in real space rotates S(Q,ω) in reciprocal space

URu_2Si_2: Phonons and magnetic excitations

NPB, et al., Physical Review B 91, 035128 (2015)

Now you're ready for a DCS experiment!

QUESTIONS?