Time-of-flight spectroscopy and the Disk Chopper Spectrometer (DCS)

www.ncnr.nist.gov/instruments/dcs

Summer School on the Fundamentals of Neutron Scattering
NIST Center for Neutron Research, June 17-21, 2013

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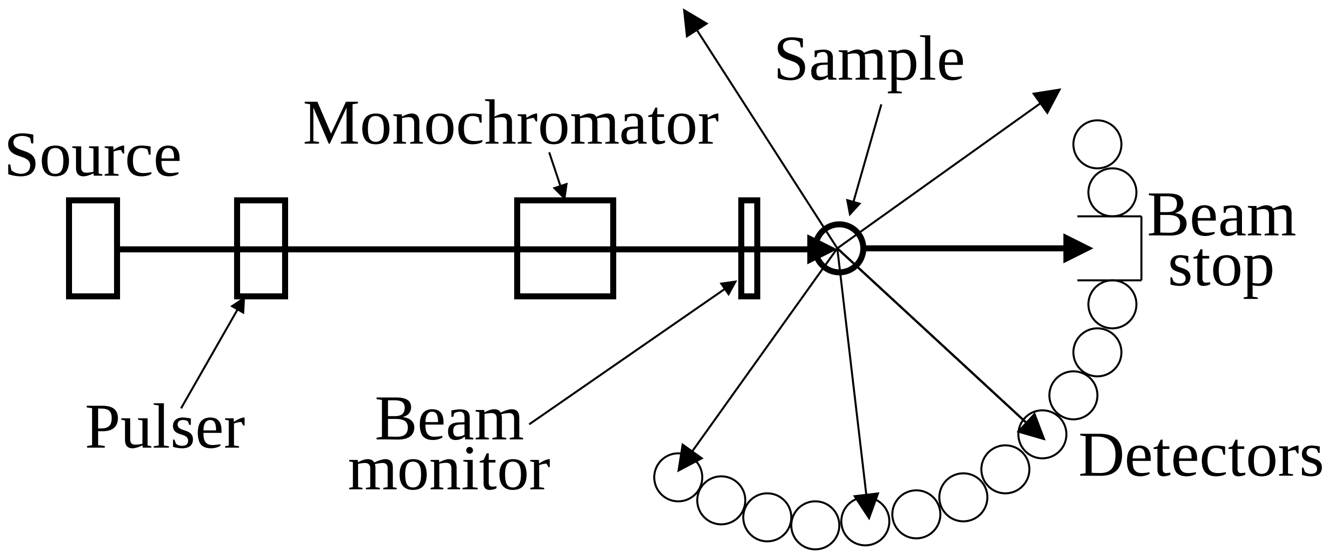
Time-of-flight spectroscopy (1)

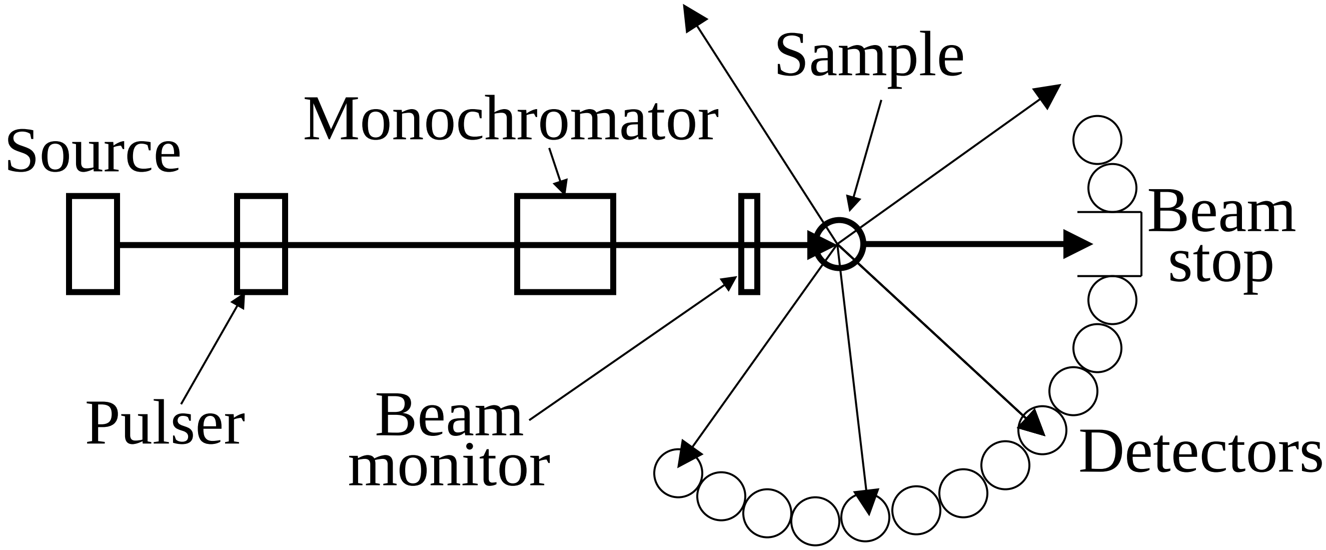


Neutrons from the source are pulsed and monochromated.

Monochromatic bursts of neutrons strike the sample.

Some of the neutrons are scattered, and some of the scattered neutrons are counted in the detectors.

Time-of-flight spectroscopy (2)



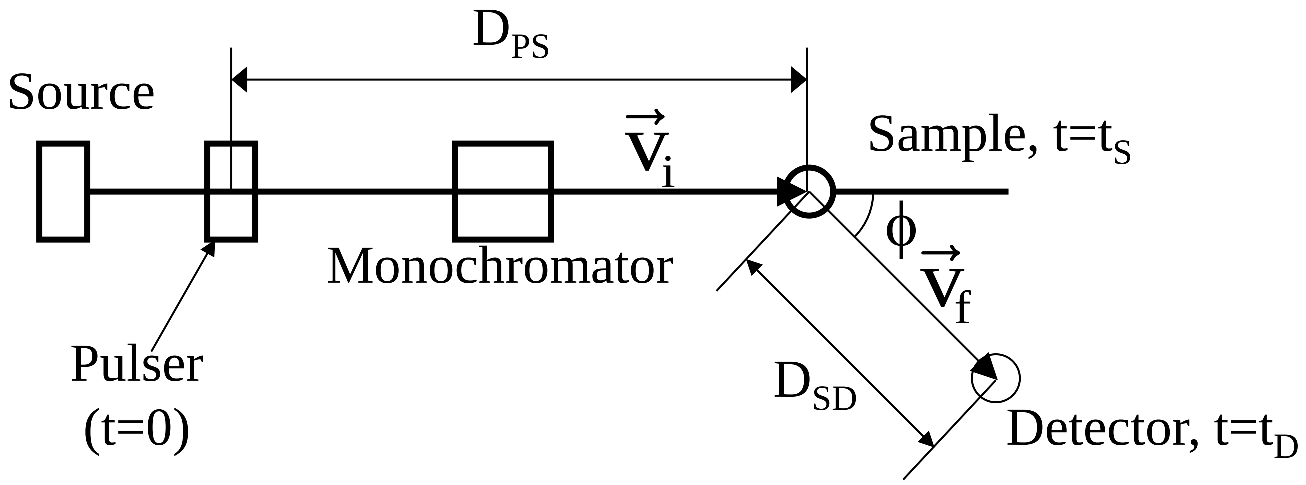
The time between pulses, T_S, is divided into 1000 time channels of width $\Delta t = 0.001 T_S$.

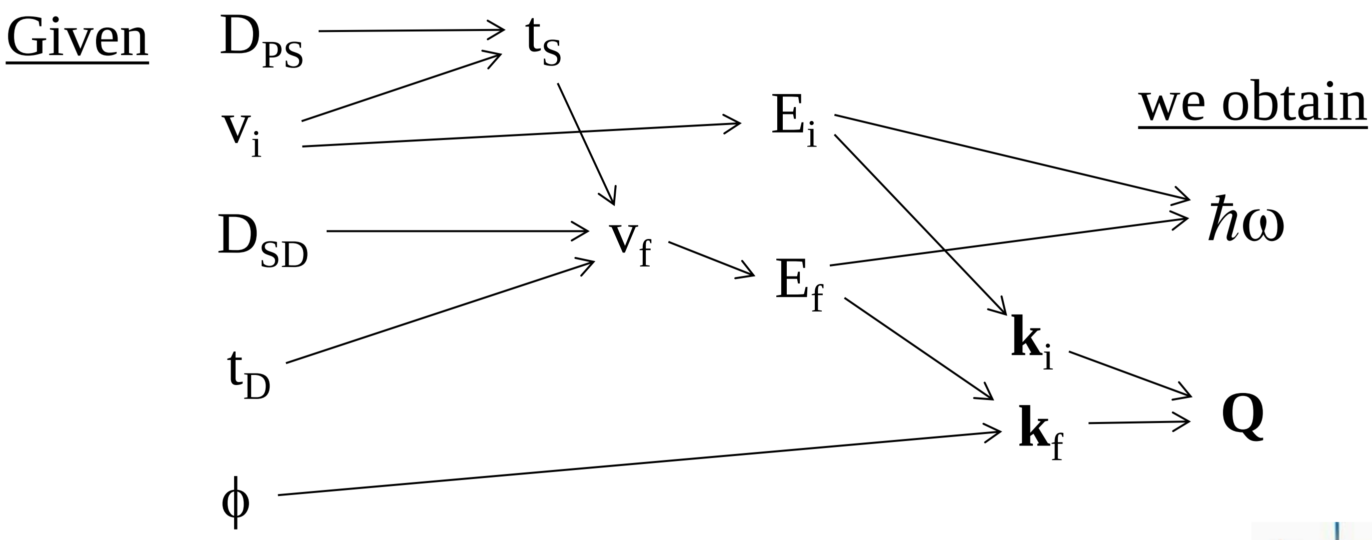
Detector events are stored in a 2-d histogram I(i,j)

i = 0…930 labels the detector, beam monitor, etc

j = 0…1023 labels the time channel

Relating t_D and ϕ to $\mathbf{Q}$ and ω





From $I(\phi,t)$ to $S(Q,\omega)$

$I(\phi,t)$ to the ddsc wrt time

Number of neutrons per second scattered at angle ϕ into solid angle $\Delta\Omega$, reaching detector within time interval $[t_D, t_D+\Delta t]$

Number of atoms of sample in the beam

Solid angle subtended by detector

Raw data

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

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

Width of time channel

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

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

To the extent that $\Delta\Omega$ and Δt are constants, $\frac{d^2\sigma}{d\Omega dt} \propto I(\phi,t)$

I(ϕ,t) to the ddsc wrt energy

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

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

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

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

I(ϕ,t) to S(Q,ω)

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

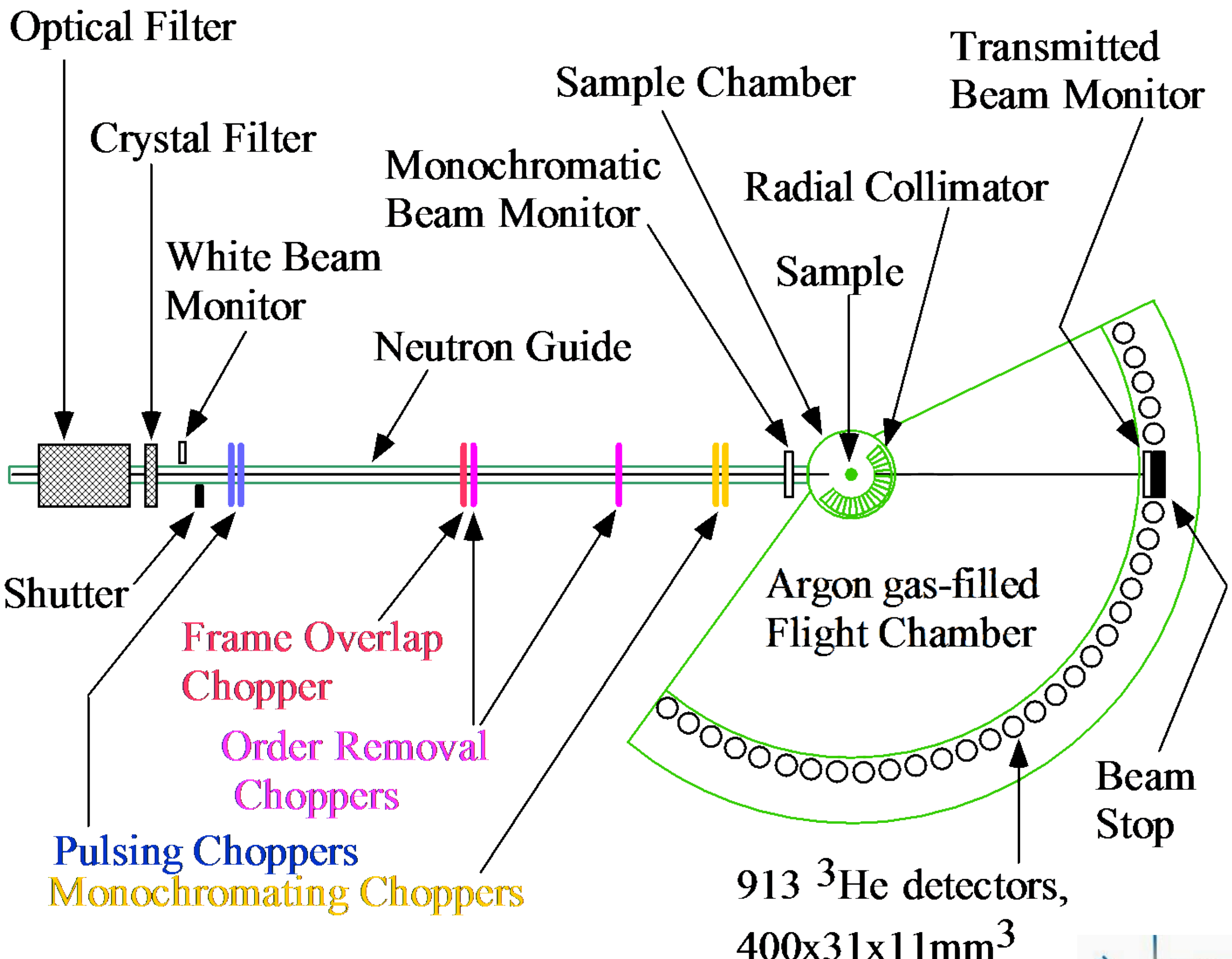
$$k_i \text{ is fixed and } k_f \propto \frac{1}{t_{SD}}$$

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

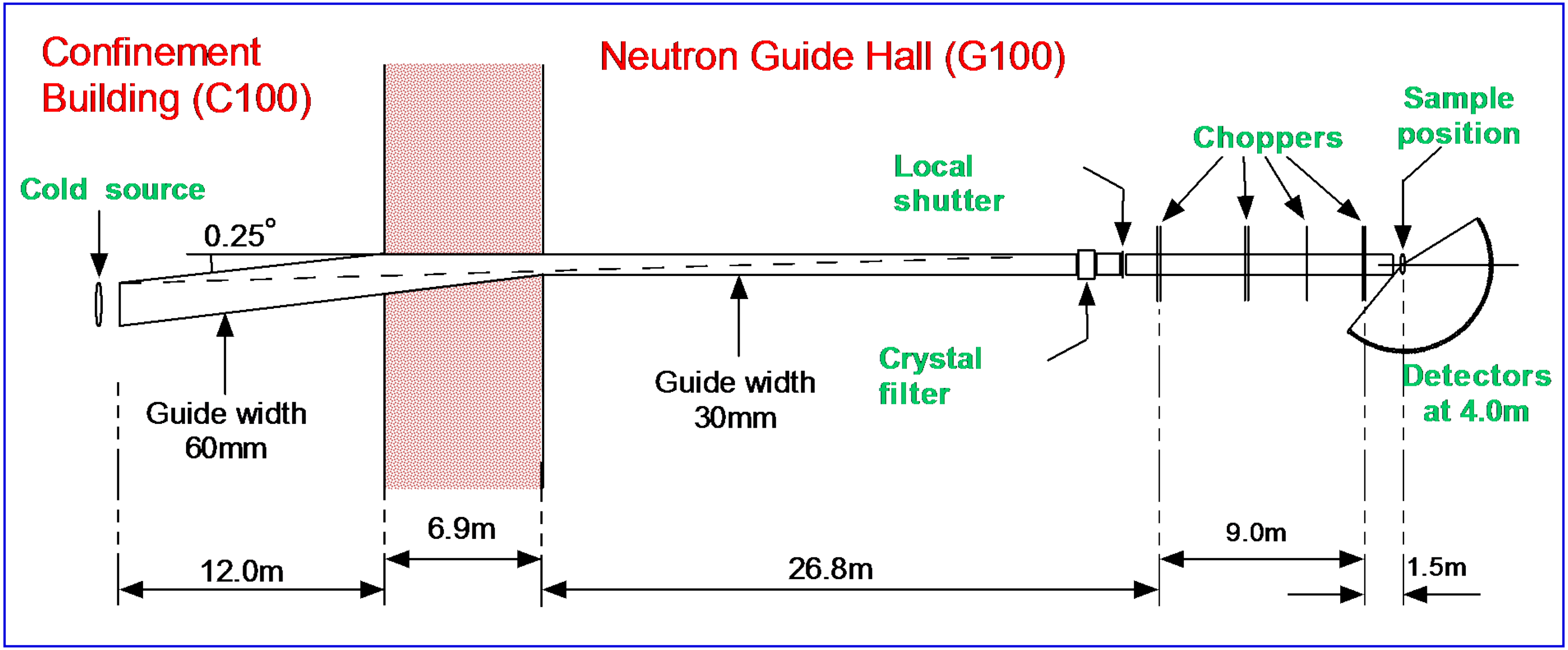
$$\boxed{\text{Hence } S(Q,\omega) \propto I(\phi,t)\cdot t_{SD}^4}$$

The Disk Chopper Spectrometer

The Disk Chopper Spectrometer - schematic



The Disk Chopper Spectrometer – plan view

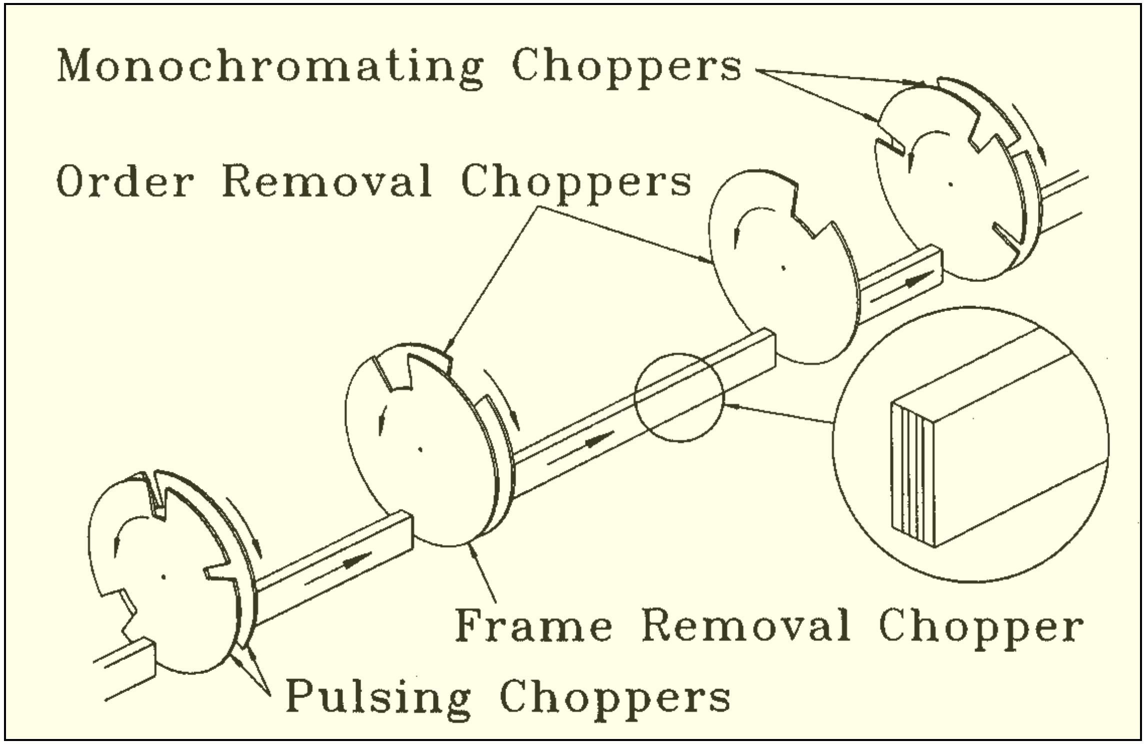


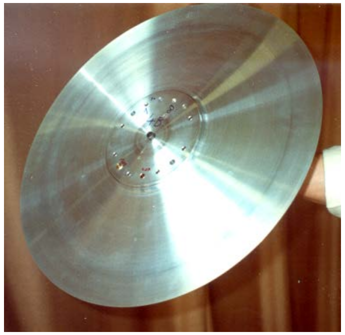
Neutron guides in the confinement building

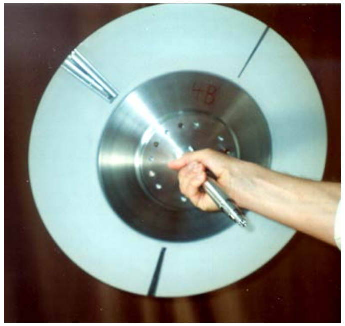
www.ncnr.nist.gov/expansion2/yqims2

13/22 (May 25 2011) From right to left, the casings for guides NG-1, 2, 3, and 4. The monolithic casing for NG-5, 6, and 7 is visible to the left.

The choppers and the guide

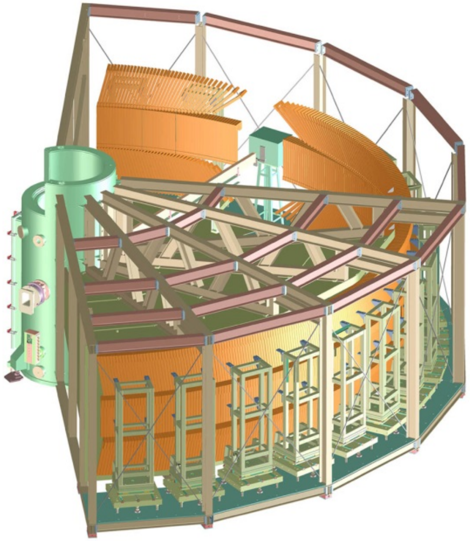






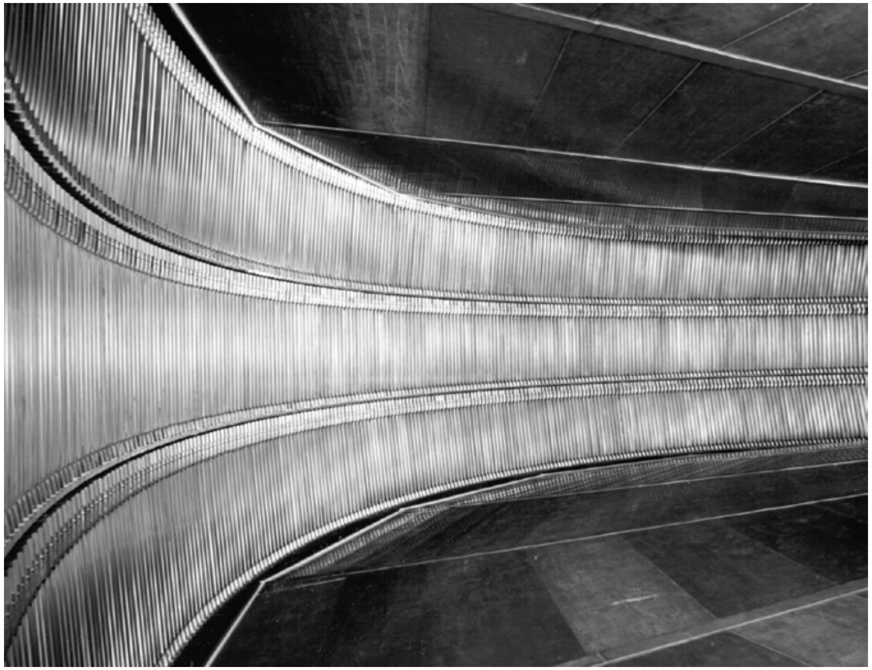
The *pulsing* and *monochromating* choppers are counter-rotating pairs, permitting a choice of pulse widths; they normally run at 20,000 rpm. The *order removal* choppers (also 20,000 rpm) remove contaminants. The *frame removal* chopper *alleviates* the problem of frame overlap. It runs at 20,000/m or 20,000(m-1)/m rpm; m is a small integer (typically m~λ/2).

The flight chamber and detectors



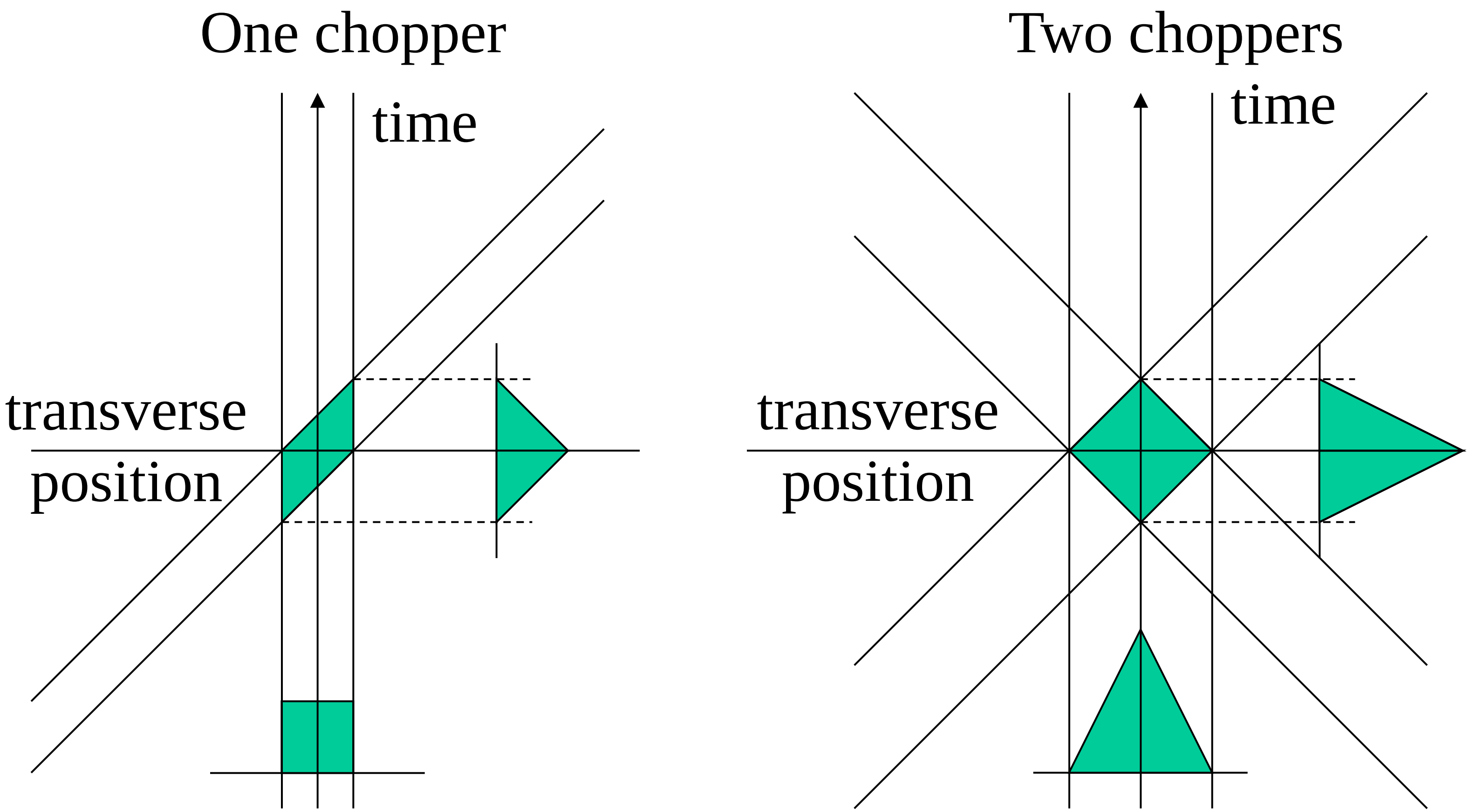
The flight chamber is argon-filled to reduce scattering of neutrons traveling the 4 m distance from sample to detectors.

There are 913 detectors in 3 banks, from -30º to +140º.



Seven choppers!

Counter-rotating choppers

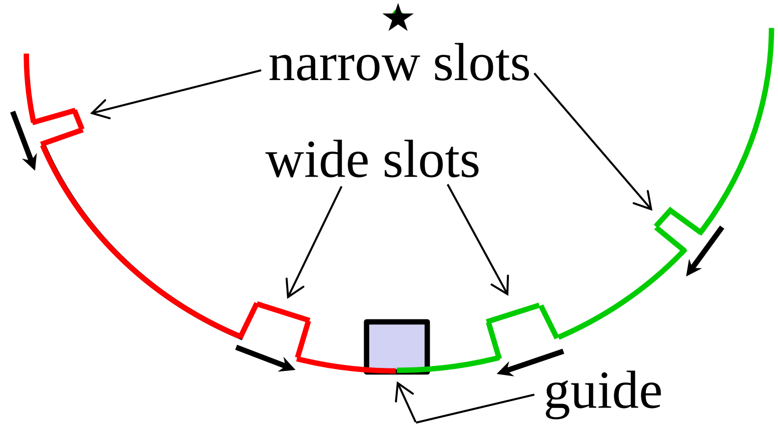


With two choppers and the same resolution width, we get twice the intensity.

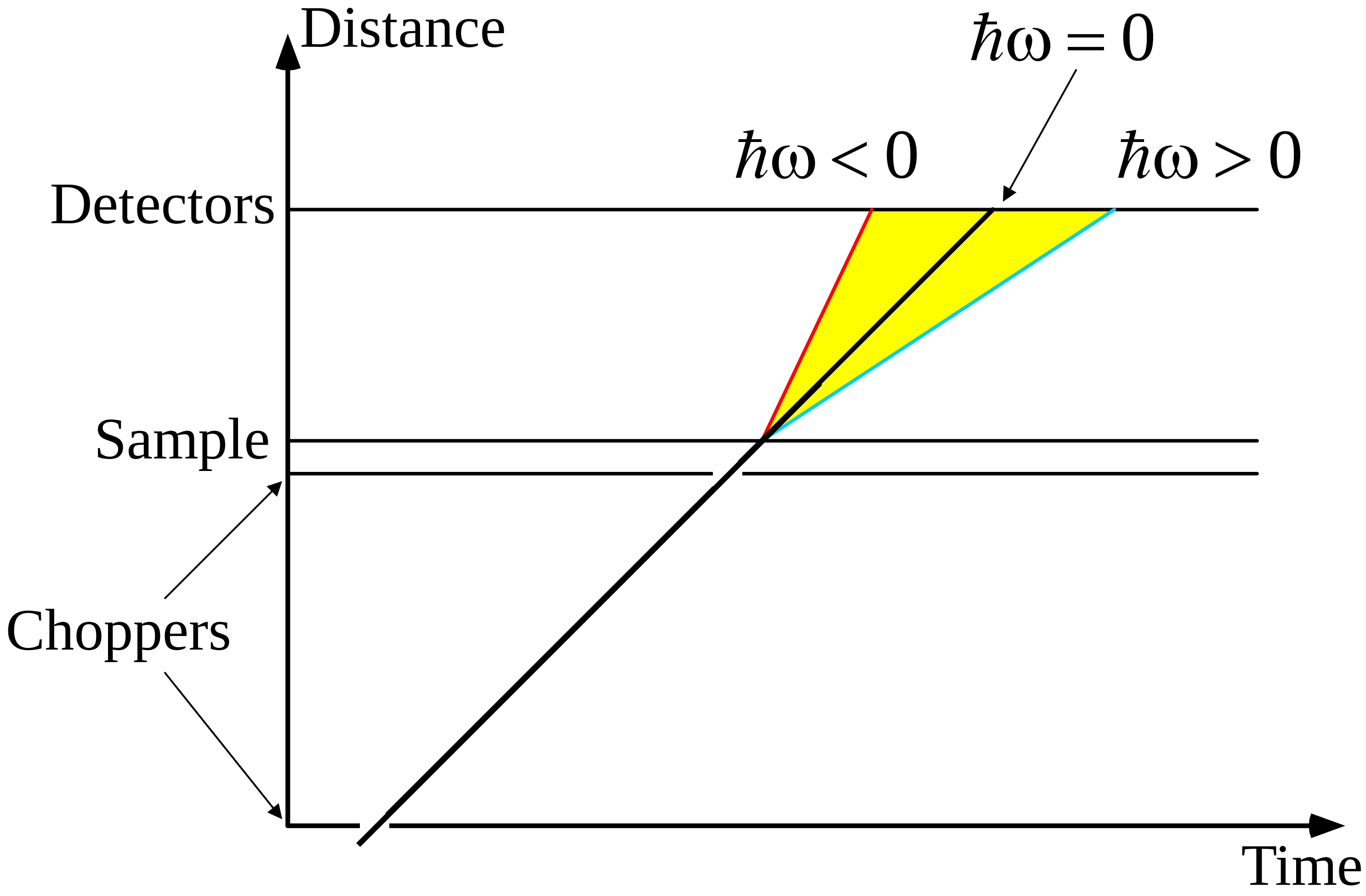
Counter-rotating choppers

By changing the relative phasing of the choppers one can arrange that selected slots, one in each chopper disk, are the only slots that line up together with the guide.

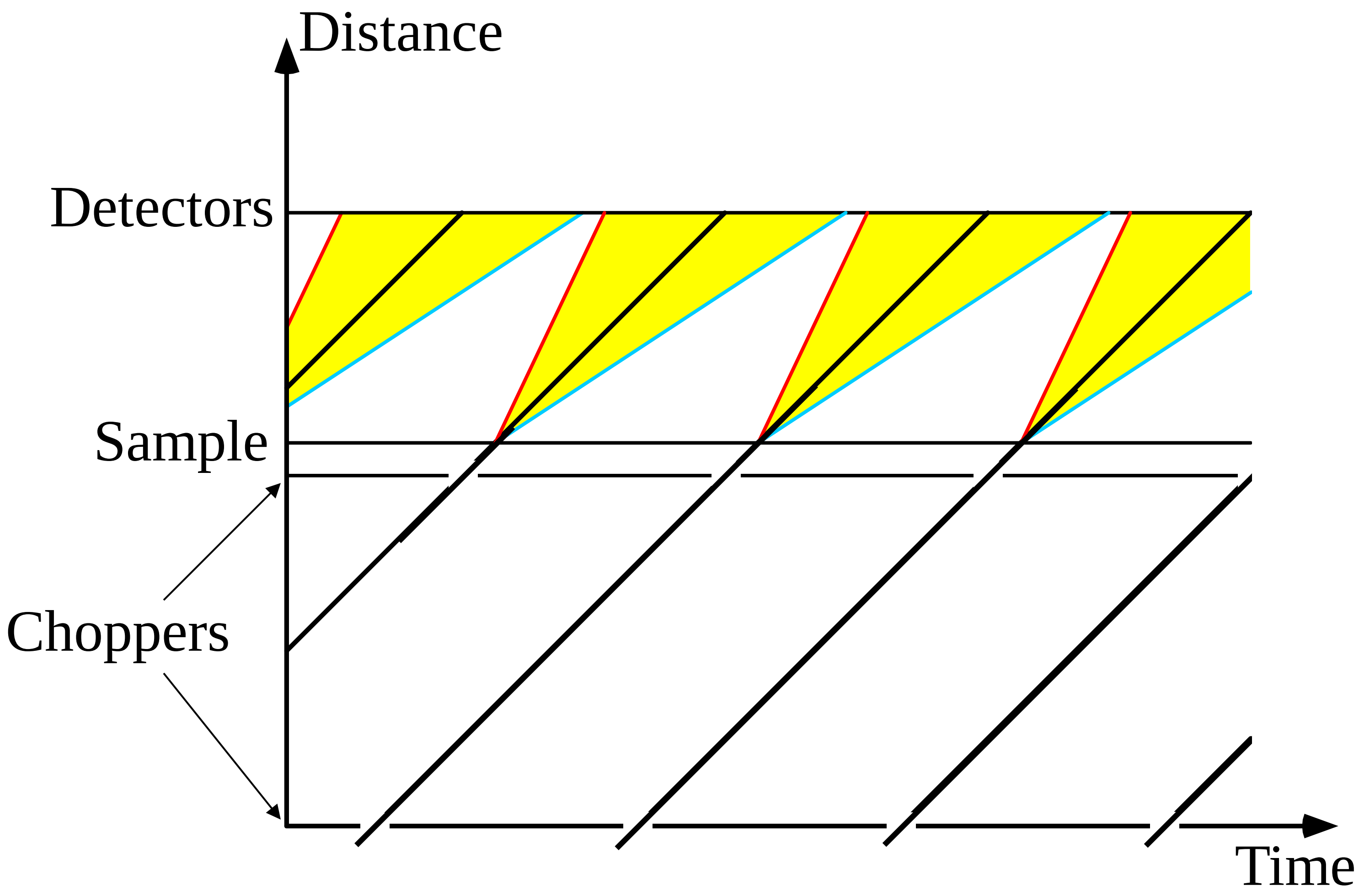
In this way the chopper burst time, and hence the instrumental resolution, can be changed without changing the wavelength or the speeds of the choppers.



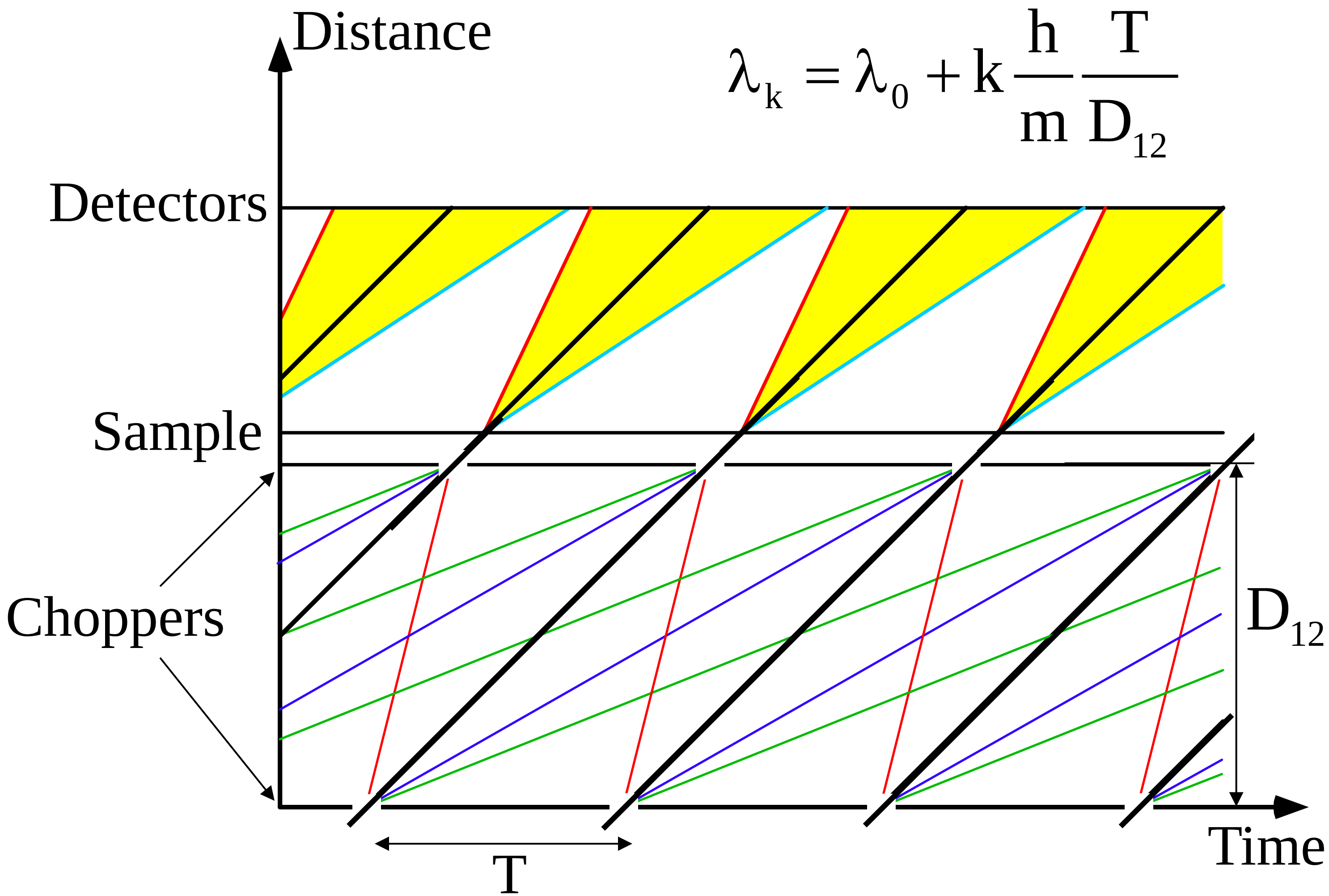
Time-distance diagrams - single pulse



Time-distance diagrams - multiple pulses



“Contaminant” wavelengths (“orders”)



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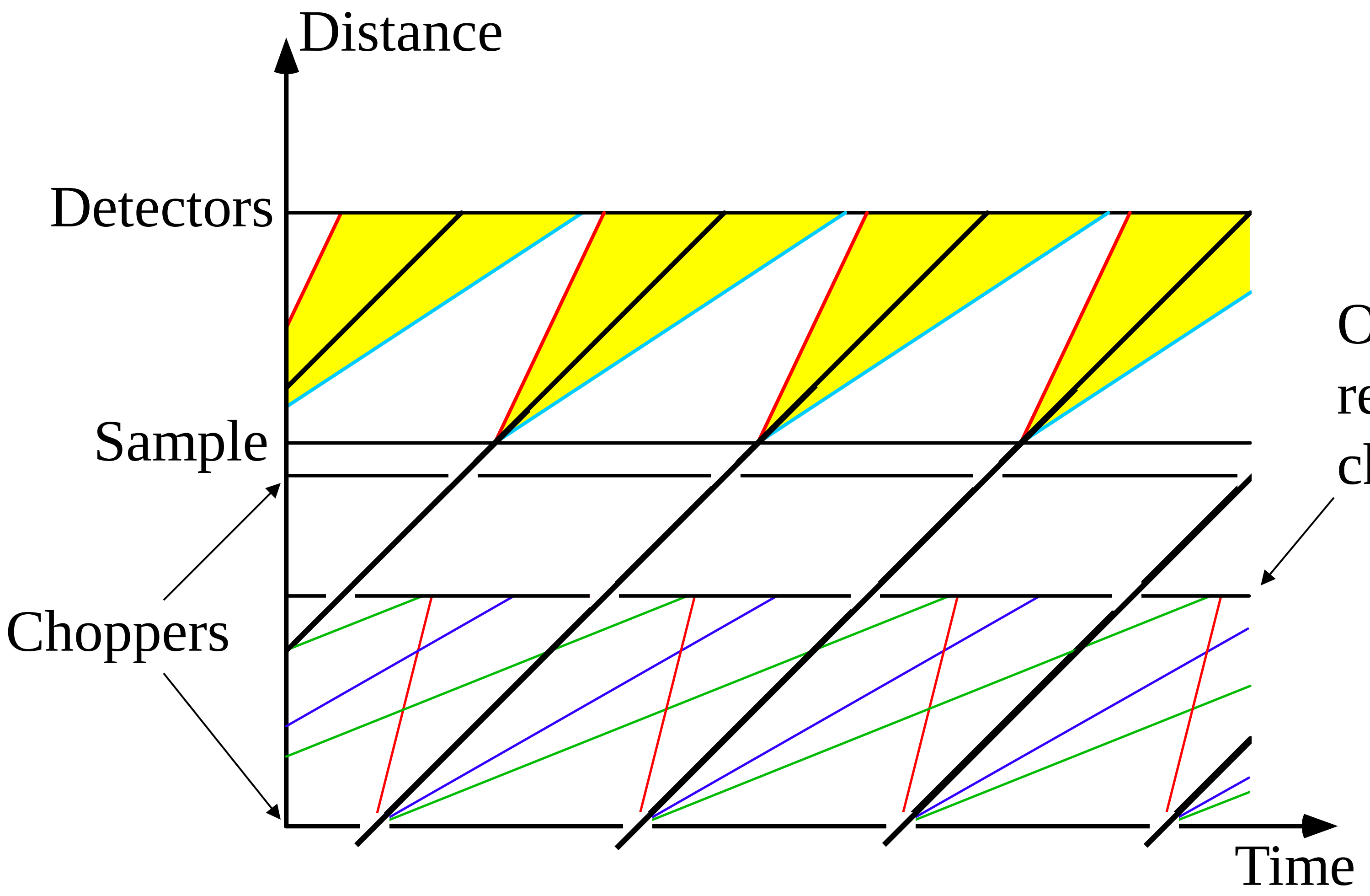
Removal of “contaminant” wavelengths



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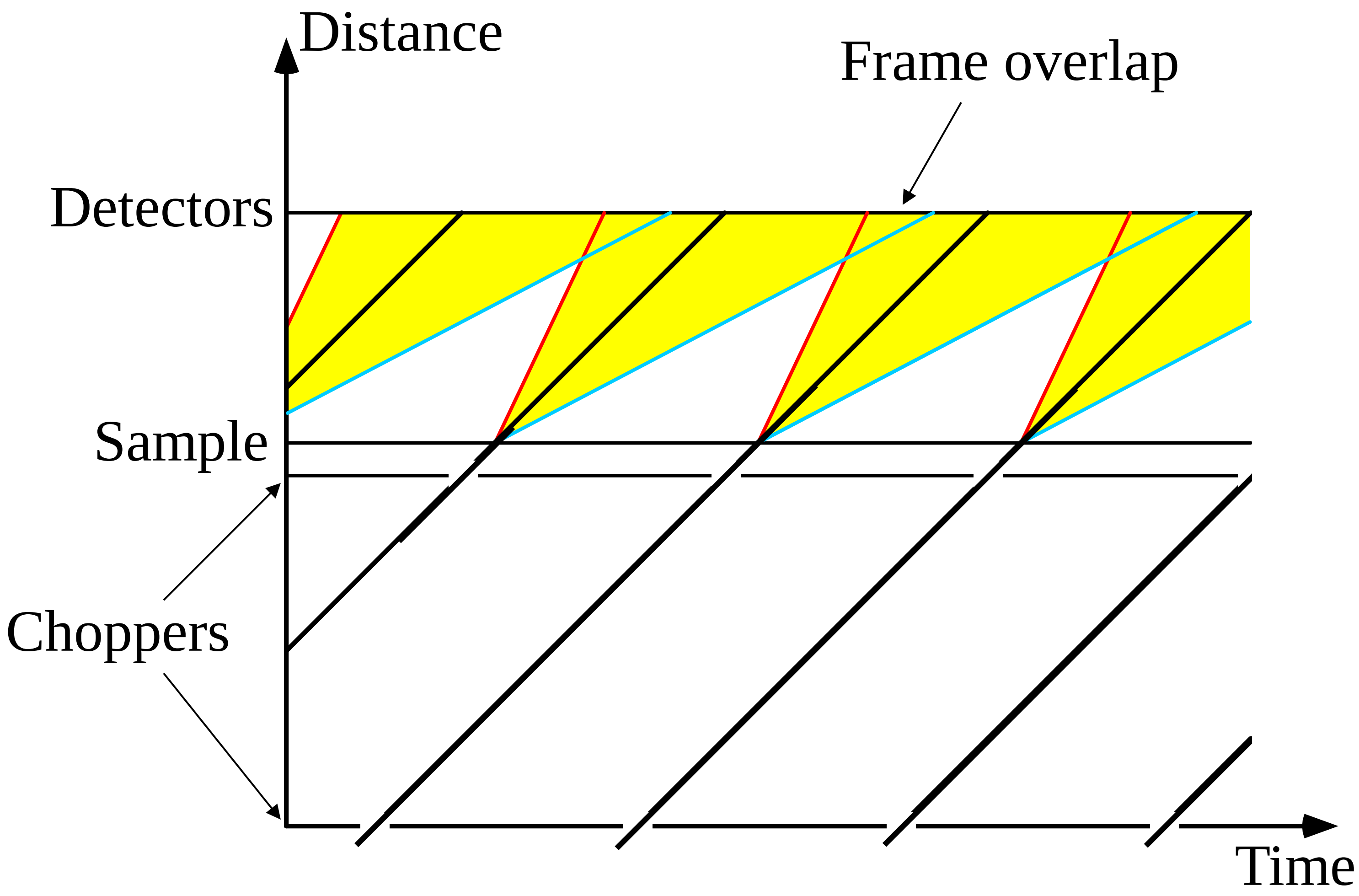
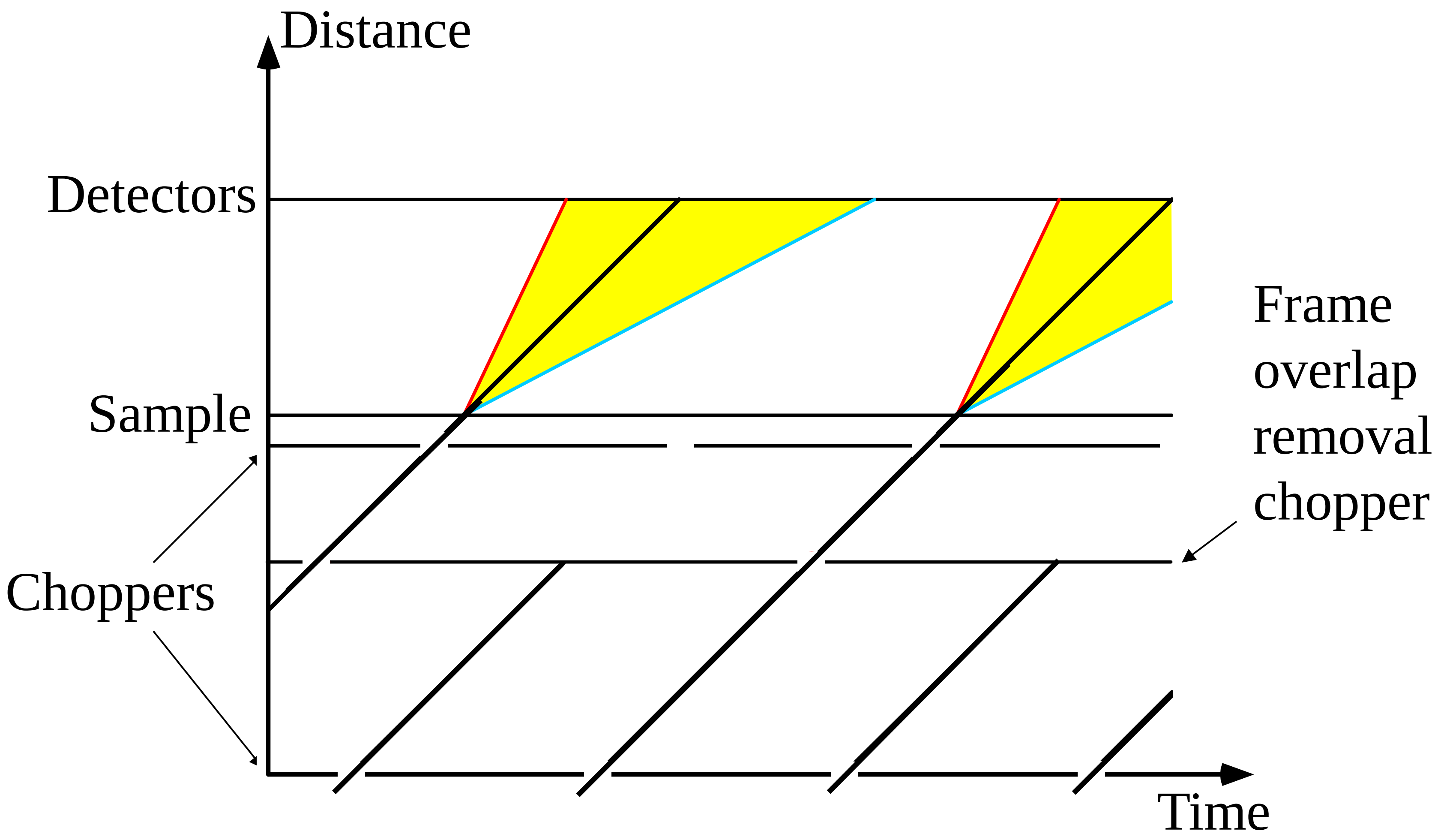
Frame overlap



Removal of frame overlap



The speed ratio denominator

The principal choppers run with period T, frequency f.

The frame overlap removal chopper runs at speed f_S=f/m where m is an integer (m can equal 1), or at f_S = f(m-1)/m, e.g. f_S/f = 1/2 or 1/3 or 2/3 or 1/4 or 3/4 ..

The time between pulses at the sample is T_S=mT.

m is called the “speed ratio denominator”.

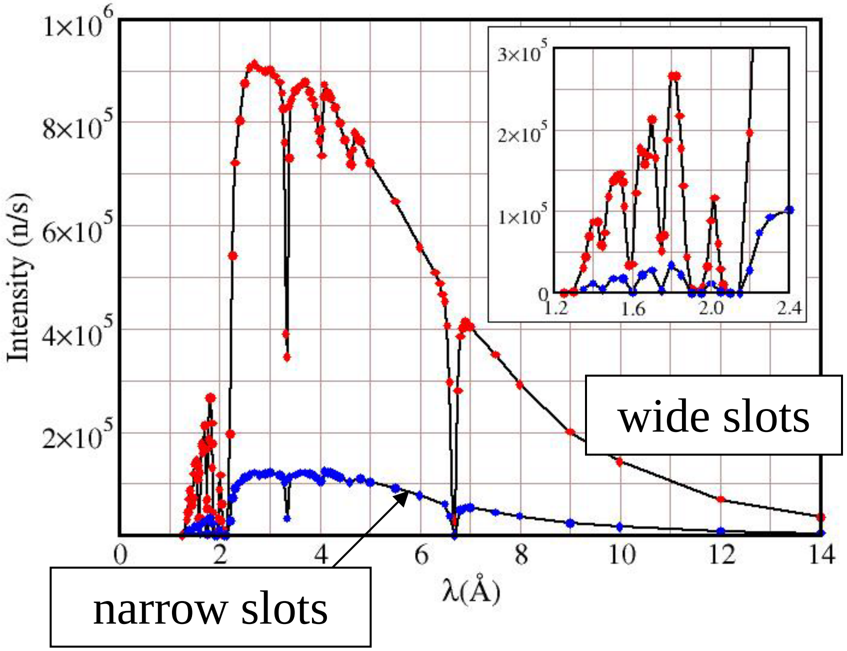
(Do not confuse this usage with m = neutron mass!)

Time

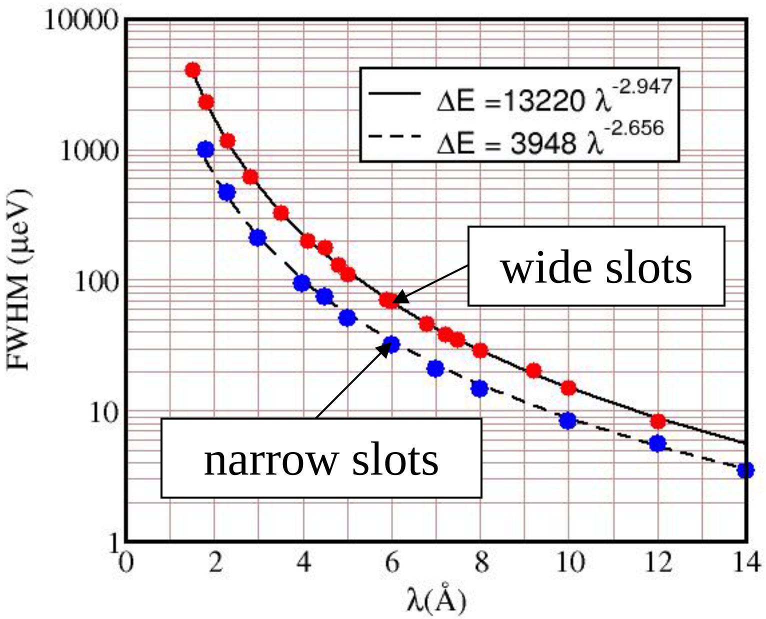
Experimental considerations

Choice of wavelength λ

Intensity at sample I(E)



Resolution width ΔE



- I(E) peaks 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 $\propto 1/\lambda$
- Bragg peaks can be troublesome at short λ (4.8Å is a popular choice)

Additional Considerations

Chopper master period T, and period at sample T_S.

- Resolution width $\Delta E \propto T$

Normally use maximum speed

- Intensity $I(E) \propto T^2/T_S = T/m$ where $m = T_S/T$ is the "speed ratio denominator"
- Thus intensity decreases with m but $\hbar\omega$ range increases (less frame overlap)

Narrow slots or wide slots?

- ΔE varies roughly as slot width W
- I(E) varies roughly as W^3

Normally use wide slots

Sample geometry

- Sample thickness: tradeoff between single and multiple scattering
- Slab, cylinder, or annular geometry?

Corrections

- Empty can; "dark count"; detector efficiency + resolution
- Self shielding