Time of Flight Inelastic Neutron Scattering

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What are my intentions in this tutorial talk?

- Purpose – explain how the Time of Flight (ToF) inelastic instruments at the SNS work
- Note: will stick specifically to SNS instruments, and will even exclude one of them (NSE)
- Keep it simple
- At SNS we have 3 classes of ToF inelastic instruments;

  (i) direct geometry

  (ii) indirect geometry

  (iii) NSE spin labeled (excluded)

OUTLINE OF TUTORIAL

The SNS itself

- How we produce neutrons, T0 timing signal
- The T0(E) and energies/timing

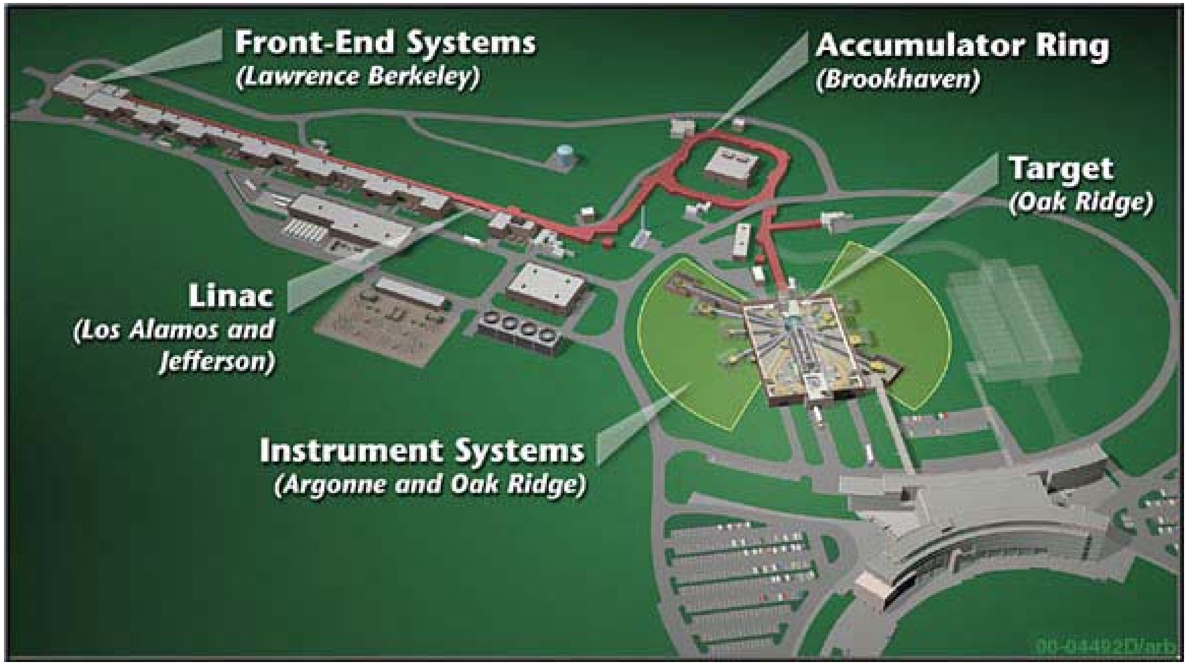
Direct geometry

- Basic principle of direct geometry
- Beamline layouts – ARCS, CNCS, SEQUOIA & HYSPEC
- T0 choppers and curved guides
- Monochromating choppers (Fermi or double disk)
- Detector tanks (vessels) and detectors (LPSD's)
- Data: detectors (LPSD), DAS, NeXus translation

Indirect Geometry

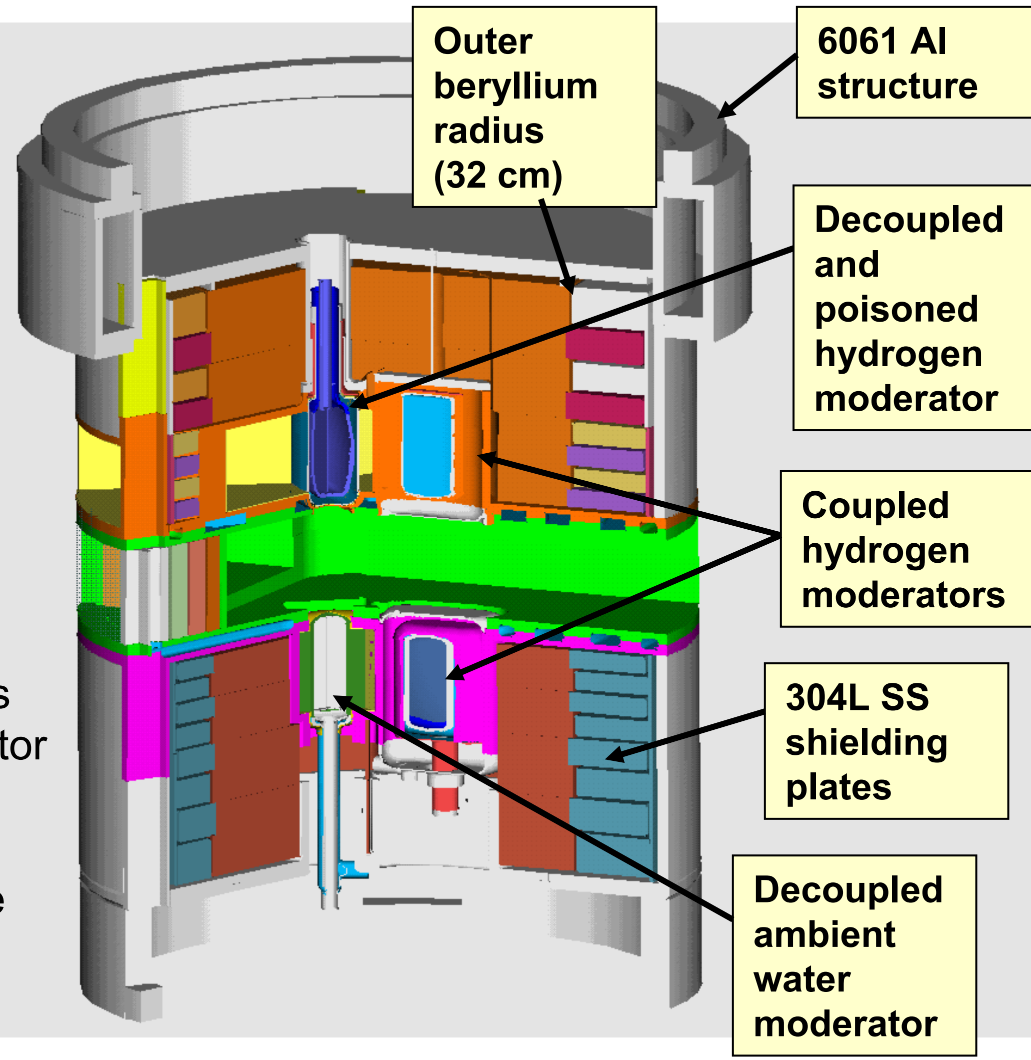
- Basic principle of indirect geometry
- Beamline layout of backscattering spectrometer BASIS
- Backscattering, long beamlines and high resolution
- Spherical analyzer panels & LPSDs – correcting for E_f variation
- Beamline layout of chemical spectrometer VISION
- HOPG analyzer panels and Be filters

The Spallation Neutron Source (SNS) at ORNL



- H^- ions are produced in the front end ion source
- H^- are accelerated to ~1GeV in Linac
- On injection into ring 2x e^- are stripped to form p
- Currently we receive a "T0" signal on injection

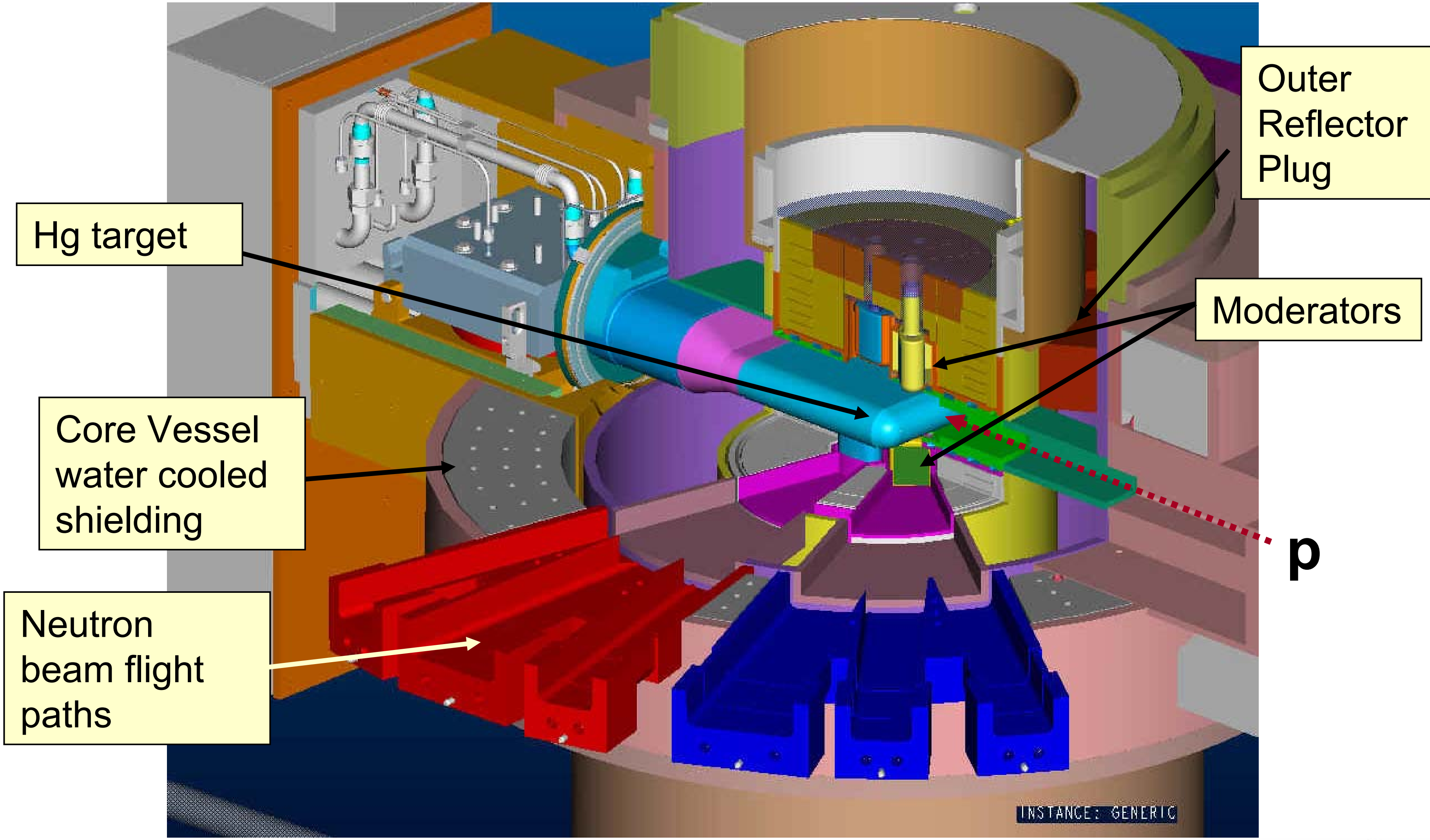
- Protons are accumulated and compressed into a 1us pulse width in the ring (~120 turns of the ring, p are traveling at ~0.9c).
- A kicker magnet knocks the proton pulse out of the ring orbit into the beamline that takes the p's to the Hg target [This is where we should in future receive the "T0" signal, on extraction.]



Inner Reflector Plug

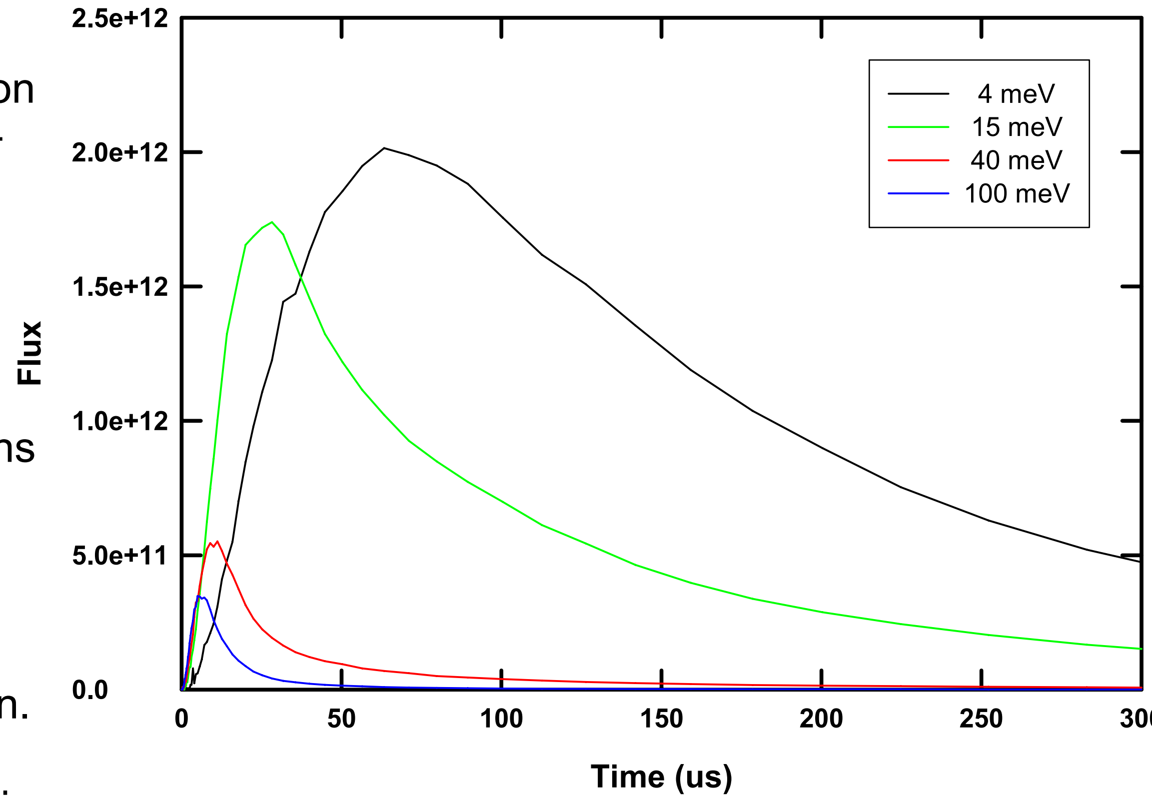
- Contains moderators and reflectors around the target. Three H moderators running at ~20K and one H_2O moderator running at 290K
- Neutrons produced by spallation in the Hg are high energy, ~1GeV, must be cooled to 1meV → 1eV range for use in thermal neutron scattering

SNS Target System

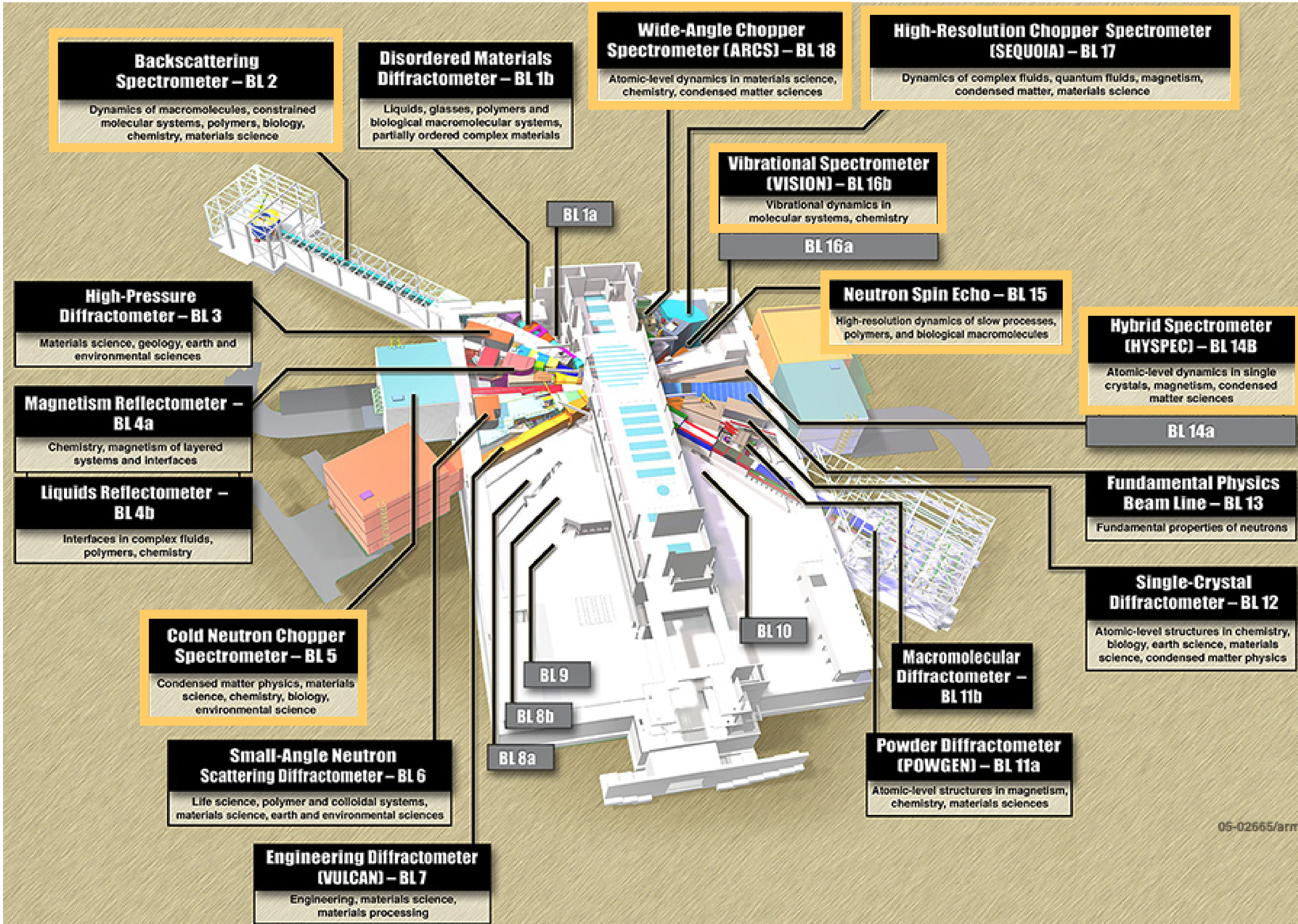


Slowing down time or T0(λ) or T0(E)

- Neutrons emerging from moderators have a distribution of energies = a Maxwellian + a 1/E (epithermal) tail.
- But different neutron energies (wavelengths) emerge from the moderator with different time distributions (see example on right).
- Need to calibrate a T0(E) function for each moderator and use this in data reduction.
- Now the neutrons are emerging out of the monolith and into the beamlines for the neutron scattering instruments…..



Example: MCNPX results for coupled cryogenic H_2 moderator on SNS target station 1



Backscattering Spectrometer – BL 2
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Disordered Materials Diffractometer – BL 1b
Liquids, glasses, polymers and biological macromolecular systems, partially ordered complex materials
Wide-Angle Chopper Spectrometer (ARCS) – BL 18
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
High-Resolution Chopper Spectrometer (SEQUOIA) – BL 17
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
BL 1a
Vibrational Spectrometer (VISION) – BL 16b
Vibrational dynamics in molecular systems, chemistry
BL 16a
High-Pressure Diffractometer – BL 3
Materials science, geology, earth and environmental sciences
Neutron Spin Echo – BL 15
High-resolution dynamics of slow processes, polymers, and biological macromolecules
Hybrid Spectrometer (HYSPEC) – BL 14B
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Magnetism Reflectometer – BL 4a
Chemistry, magnetism of layered systems and interfaces
BL 14a
Liquids Reflectometer – BL 4b
Interfaces in complex fluids, polymers, chemistry
Fundamental Physics Beam Line – BL 13
Fundamental properties of neutrons
Single-Crystal Diffractometer – BL 12
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
BL 10
Cold Neutron Chopper Spectrometer – BL 5
Condensed matter physics, materials science, chemistry, biology, environmental science
BL 9
Macromolecular Diffractometer – BL 11b
BL 8b
BL 8a
Small-Angle Neutron Scattering Diffractometer – BL 6
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
Powder Diffractometer (POWGEN) – BL 11a
Atomic-level structures in magnetism, chemistry, materials sciences
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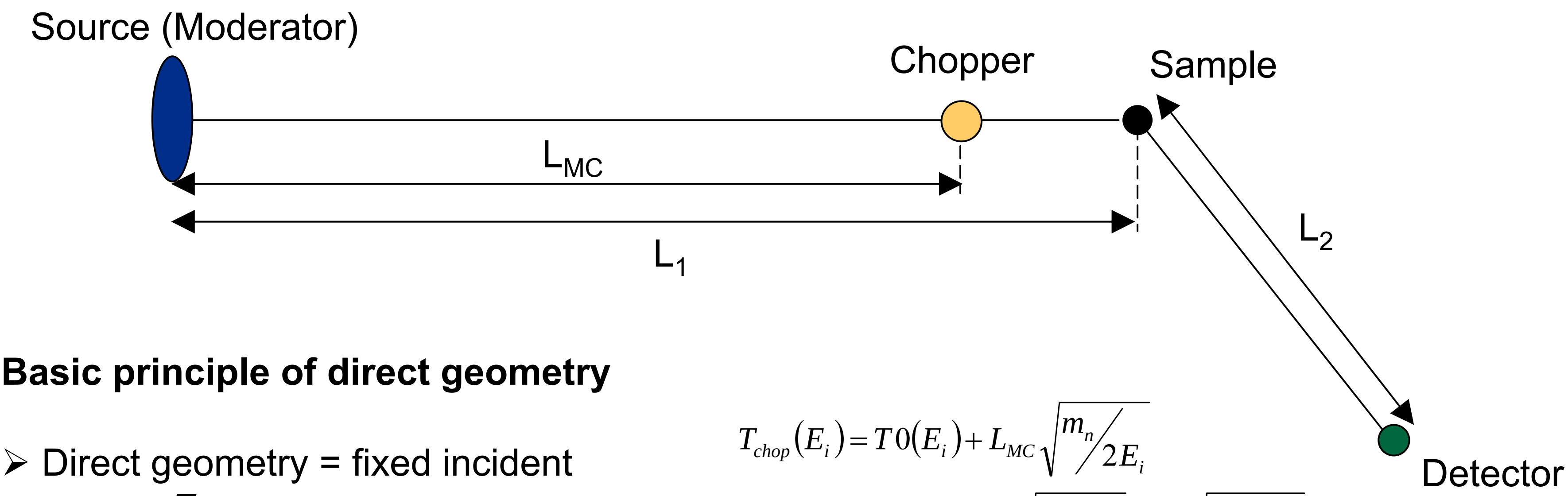
Engineering Diffractometer (VULCAN) – BL 7
Engineering, materials science, materials processing

DIRECT GEOMETRY



Basic principle of direct geometry

- Direct geometry = fixed incident energy E_i
- The chopper opens at time T_{chop} to let one energy E_I pass through
- At the sample neutrons with energy E_i transfer energy E to the sample and emerge with final energy E_f
- After scattering neutrons are measured in the detector at time $T_{detector}$.

$$T_{chop}(E_i) = T0(E_i) + L_{MC}\sqrt{m_n/2E_i}$$

$$T_{detector} = T0(E_i) + L_1\sqrt{m_n/2E_i} + L_2\sqrt{m_n/2E_f}$$

$$E_f = \frac{1}{2}m_n\left(\frac{L_2}{T_{detector} - T0(E_i) - L_1\sqrt{m_n/2E_i}}\right)^2$$

$$E = E_i - E_f$$

$$= E_i - \frac{1}{2}m_n\left(\frac{L_2}{T_{detector} - T0(E_i) - L_1\sqrt{m_n/2E_i}}\right)^2$$

Resolution (qualitative – not M.C.)

τ_M – source (moderator) pulse width for E_I

Δt_C – burst time for Fermi chopper

Primary spectrometer

$$\frac{\Delta E_I}{E_I} = 2\frac{\Delta T_I}{T_I} = 2\frac{\sqrt{(\tau_M)^2 + (\Delta t_C)^2}}{T_{MC}} = \frac{\sqrt{(\tau_M)^2 + (\Delta t_C)^2}}{1142\ L_{MC}}\sqrt{E_I}$$

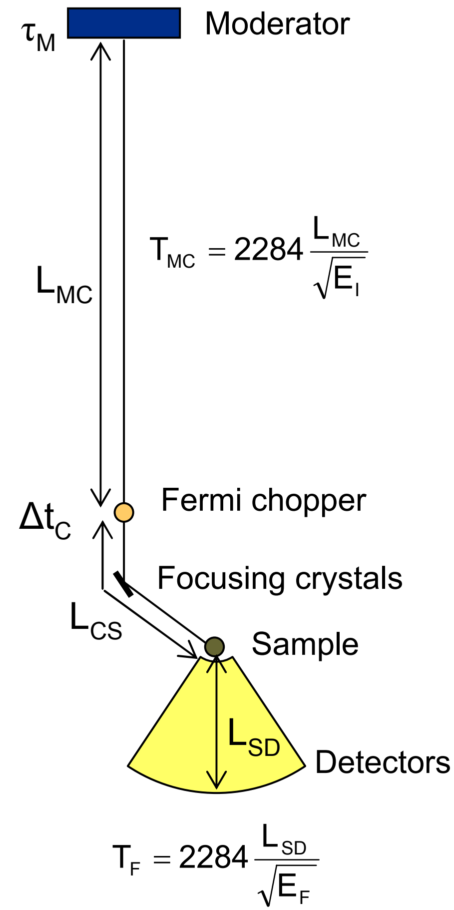
- Low E_I – τ_M dominates
- High E_I – Δt_C dominates

Secondary spectrometer

$$\frac{\Delta E_F}{E_F} = 2\frac{\Delta T_S}{T_F} = \frac{\Delta t_C}{1142\ \ L_{SD}}\left[1+\left(\frac{L_{CS}}{L_{MC}}\right)^2\left(1+\frac{\tau_M^2}{\Delta t_C^2}\right)\right]^{1/2}\sqrt{E_F}$$

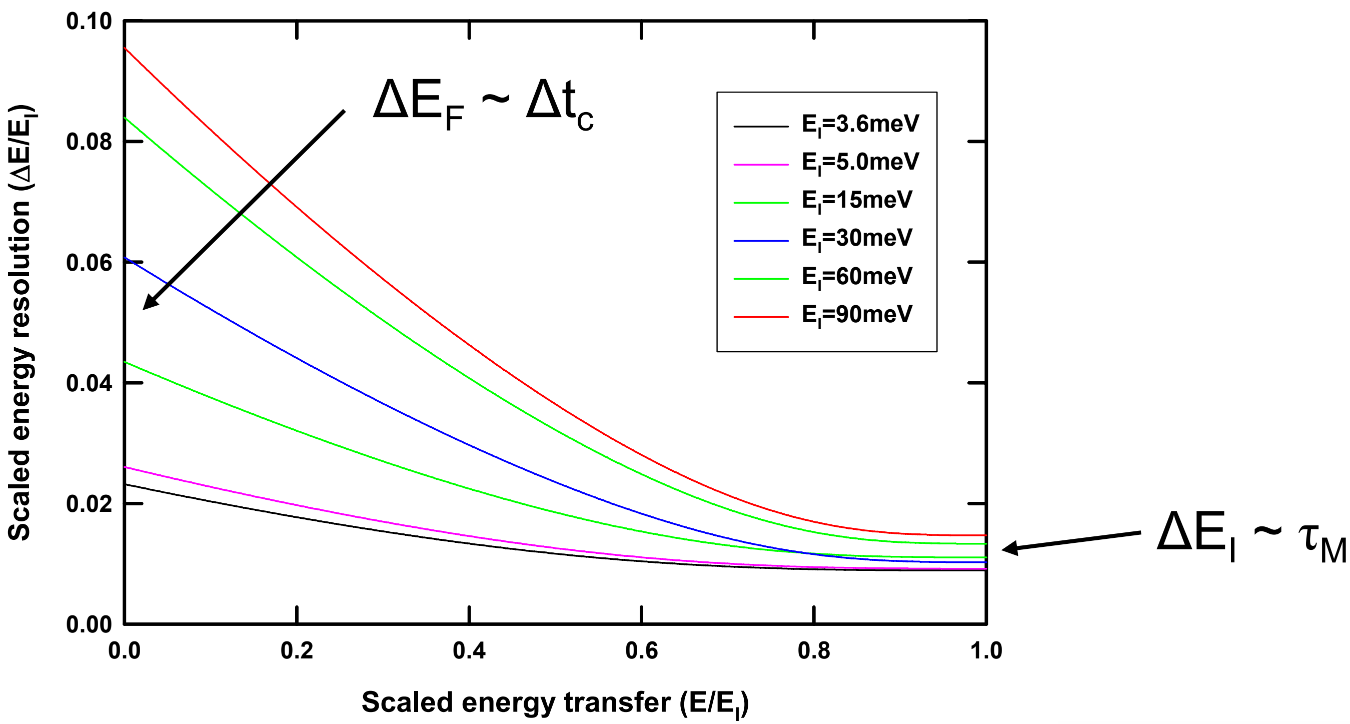
Spreading of pulse from chopper to sample

Secondary resolution governed by ratio
of burst time Δt_C to distance L_{SD}

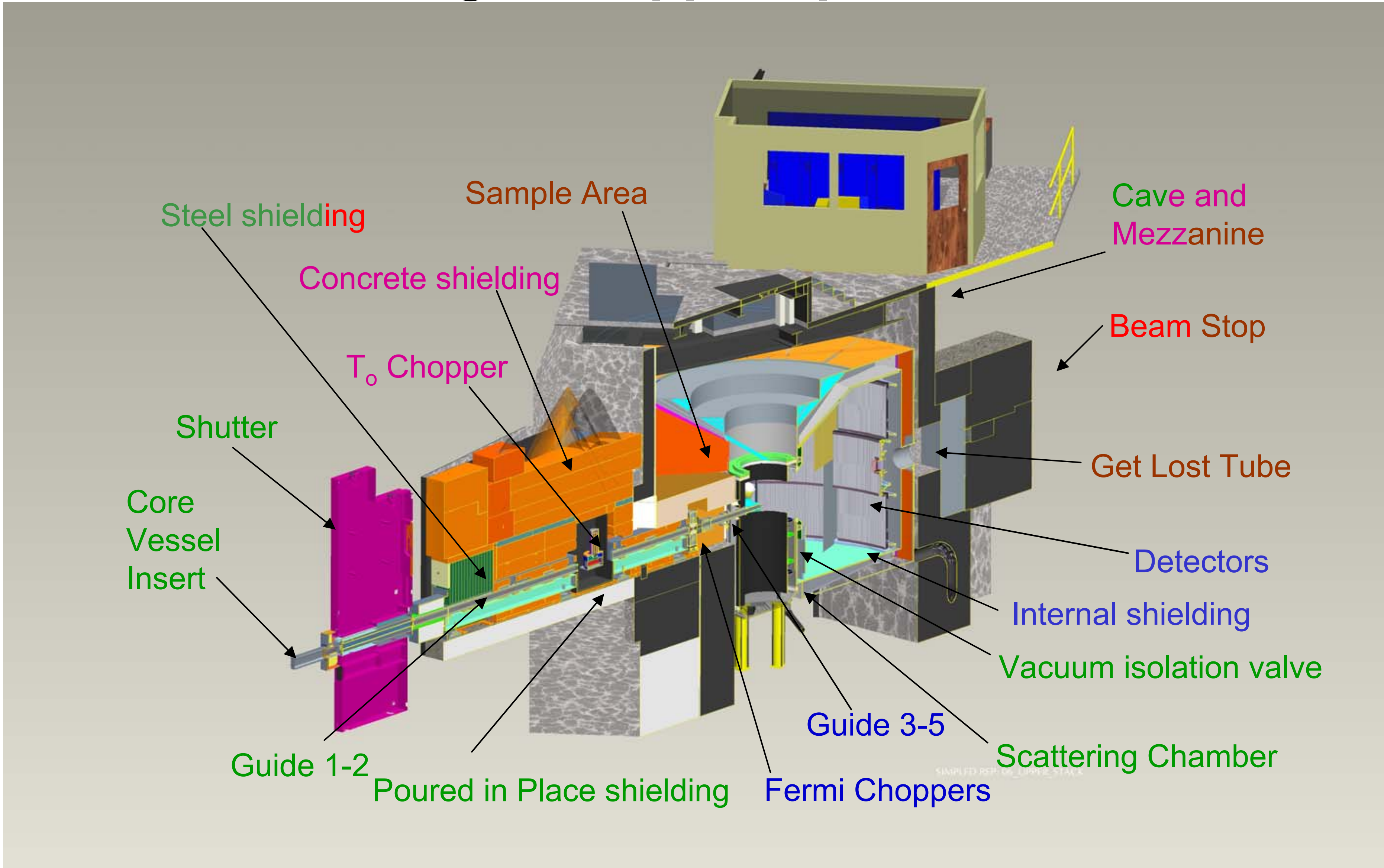


$$\Delta E = \sqrt{(\Delta E_I)^2 + (\Delta E_F)^2}$$

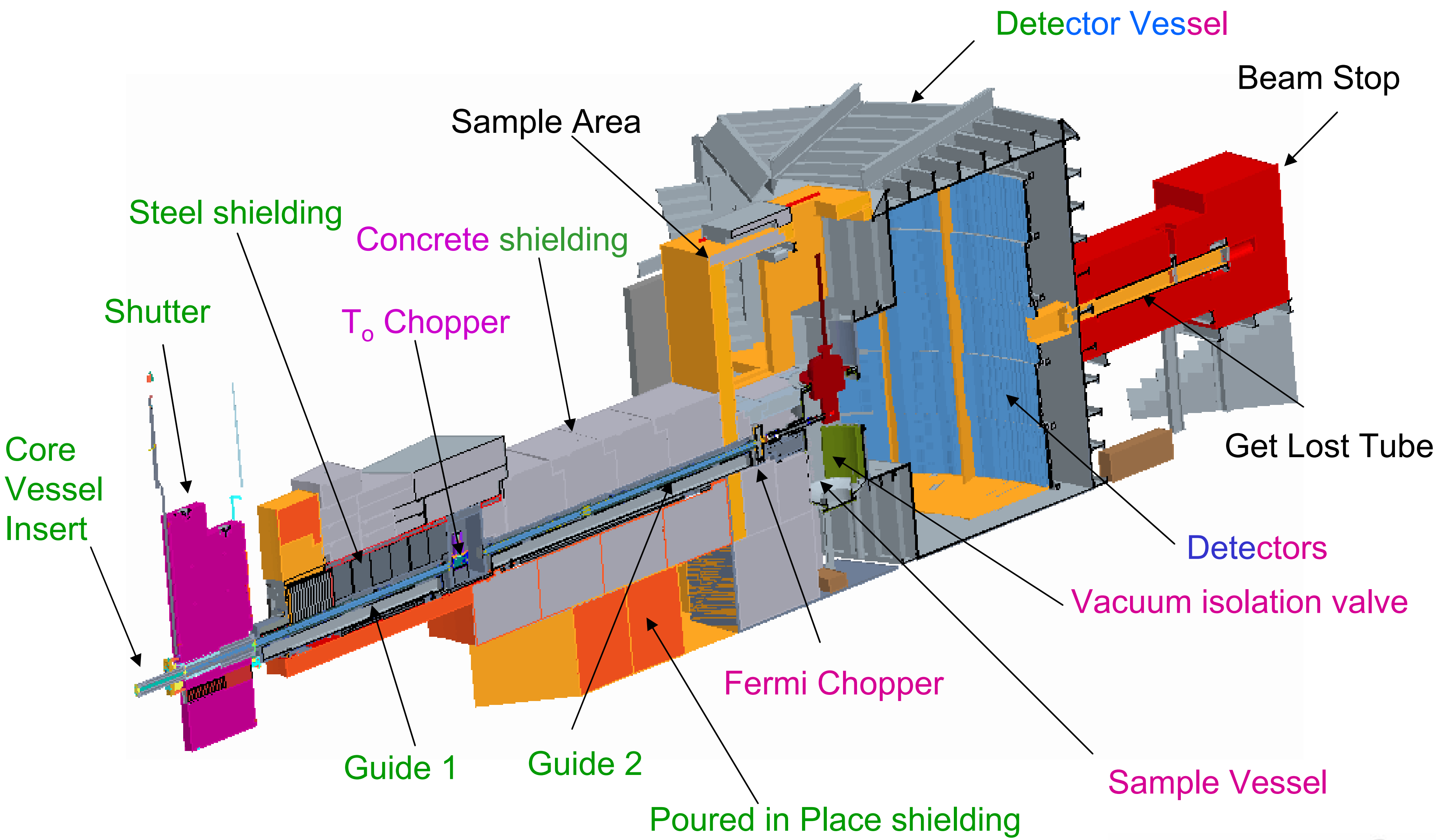
$$= \frac{1}{1142}\sqrt{\left(\frac{\tau_M^2 + \Delta t_C^2}{L_{MC}^2}\right)E_I^3 + \left(\frac{\Delta t_C}{L_{SD}}\right)^2\left[1 + \left(\frac{L_{CS}}{L_{MC}}\right)^2\left(1 + \frac{\tau_M^2}{\Delta t_C^2}\right)\right]E_F^3}$$



ARCS – wide angle chopper spectrometer

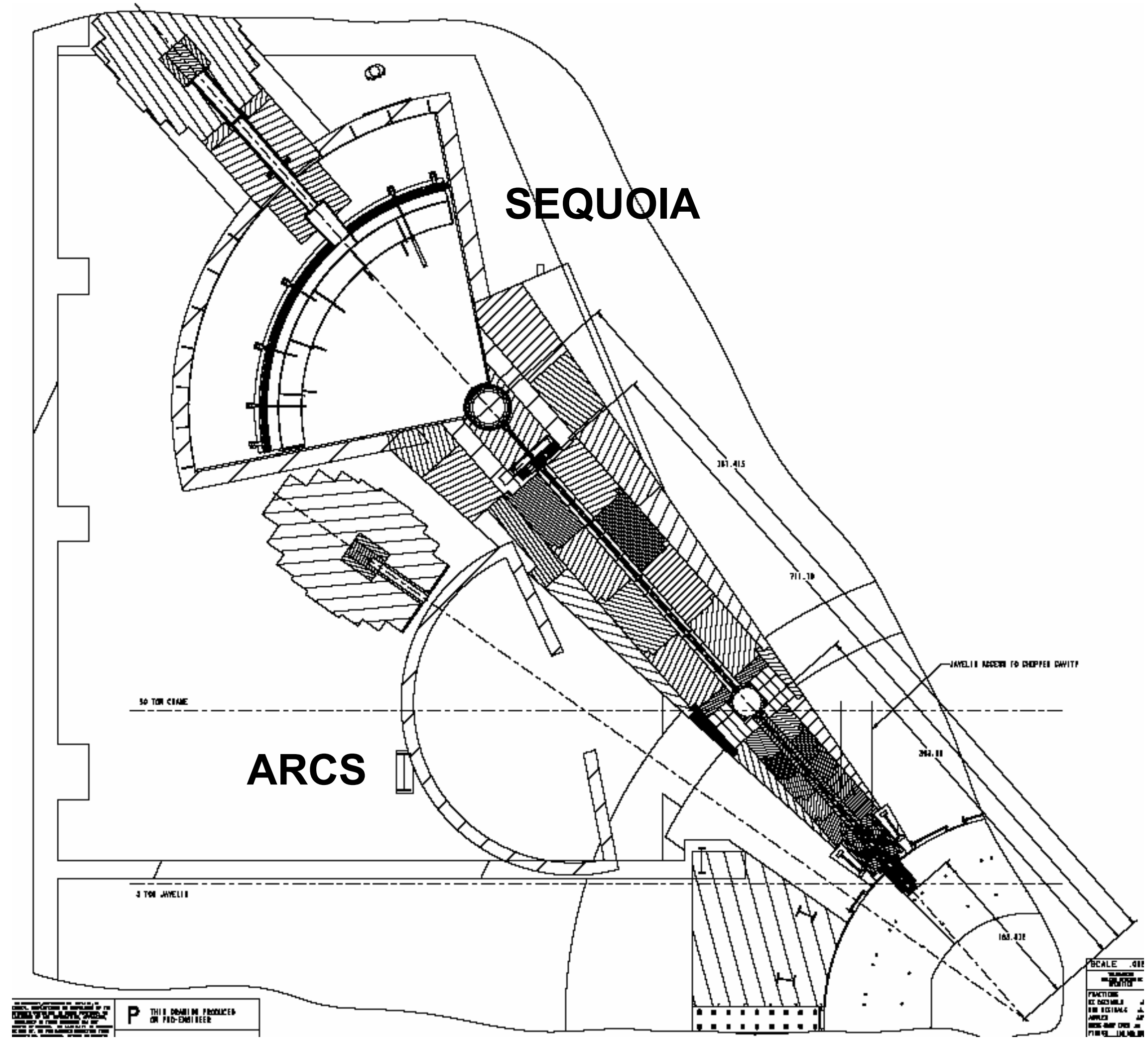


SEQUOIA – high resolution chopper spectrometer



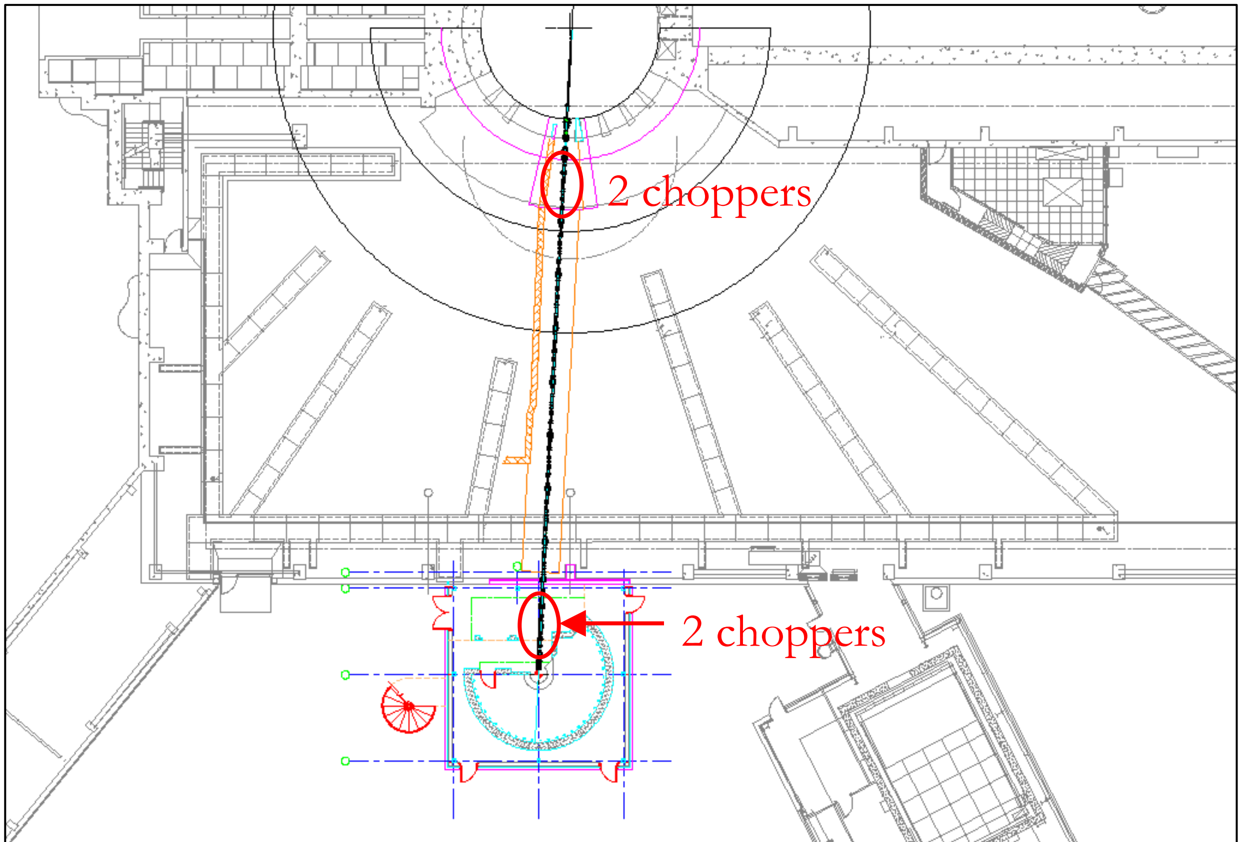
ARCS and SEQUOIA

- Closely related, both physically on BL17 and BL18 and also in terms of parameters and science.
- Both have incident energy range of nominally 10meV → 1.5eV (better at ~100meV and above)
- SEQUOIA optimized for magnetic inelastic scattering (in forward direction), which falls off with increasing Q (angle).
- ARCS optimized for phonon scattering, which increases with increasing Q (angle).

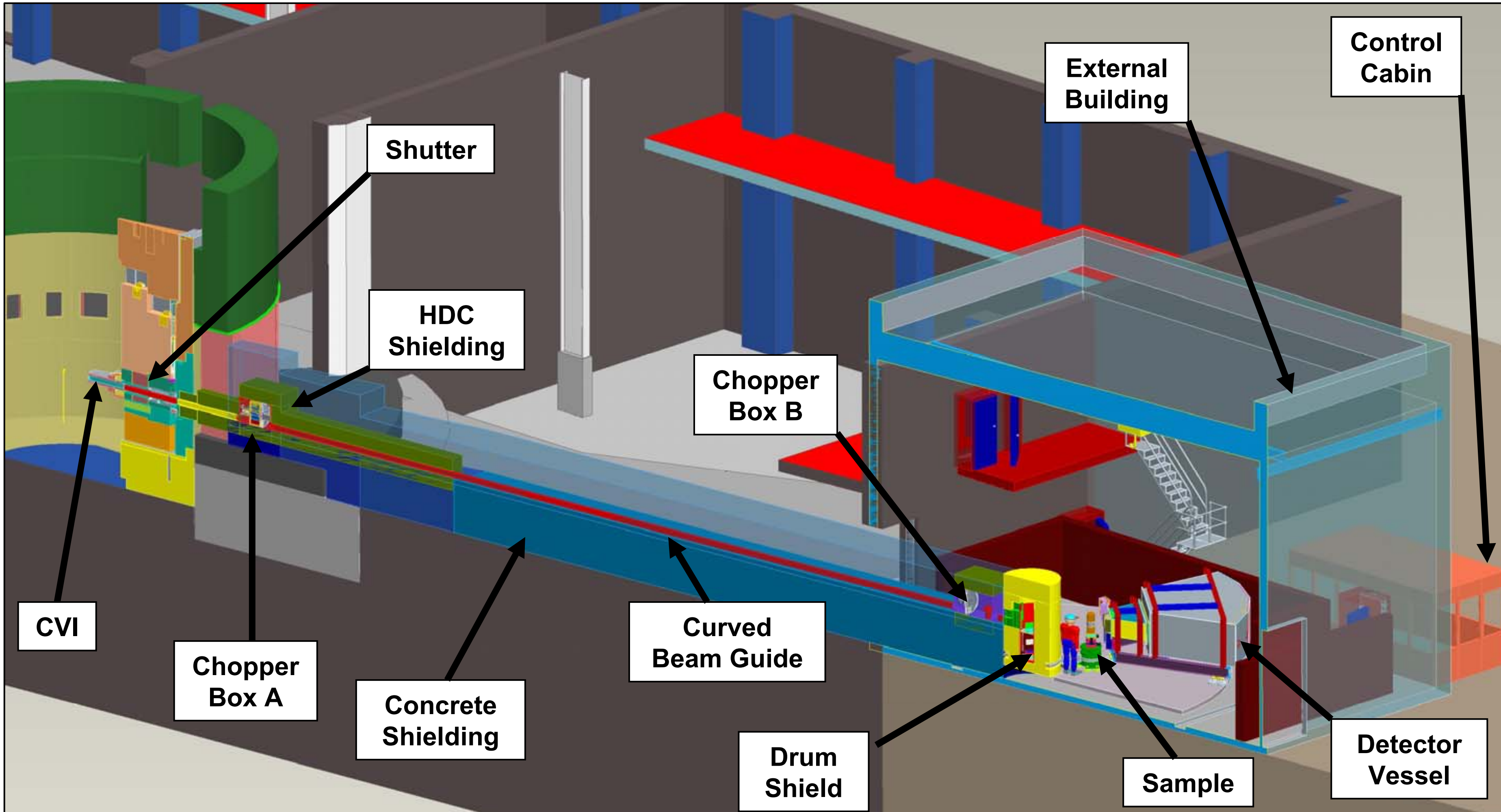


CNCS – cold neutron chopper spectrometer

Incident neutrons	E_i = 2-50 meV	Source to sample distance	36.2 m
	λ_i = 1.5-10 Å	Moderator	coupled cryo-H_2
Resolution	ΔE = 10-500 μeV	Sample to detector distance	3.5 m
		Detector coverage	-90 ... +140° (horz) ± 25° out of plane

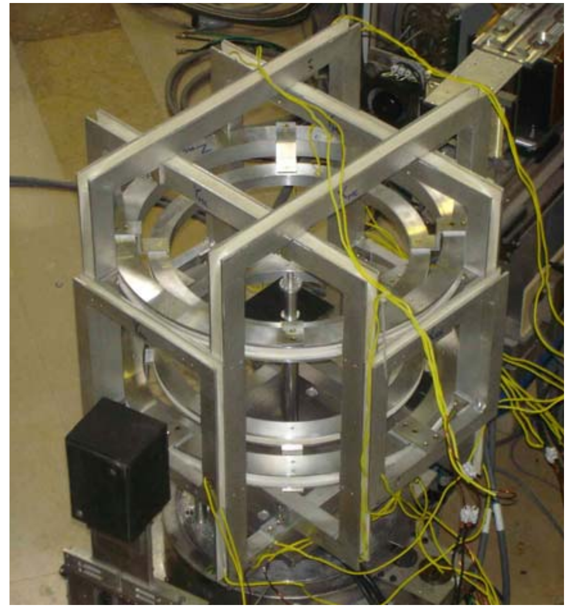


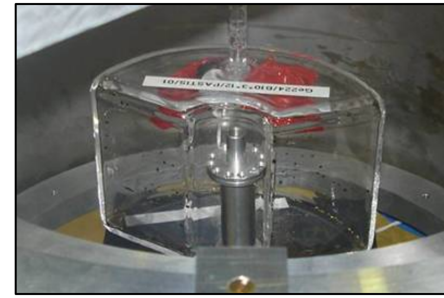
HYSPEC – polarized beam spectrometer

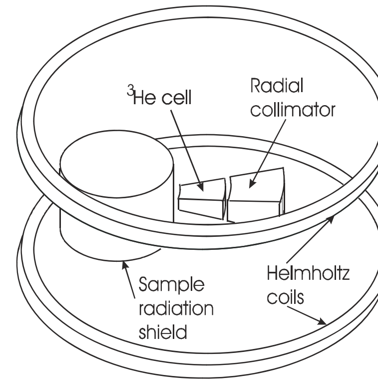


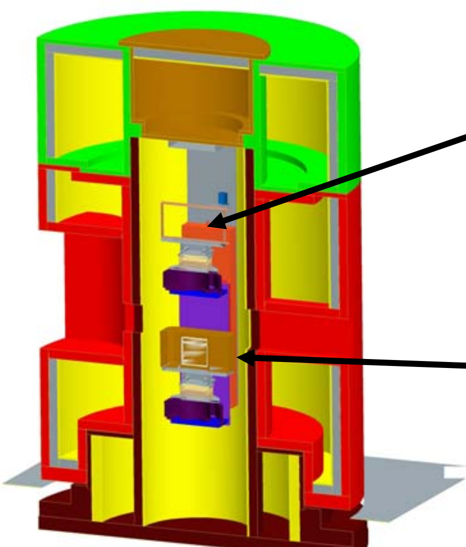
HYSPEC – Focusing & Polarizing

- Optimized for single crystals & "in-plane" scattering
- Can deploy polarizers and analyzers for neutron spin





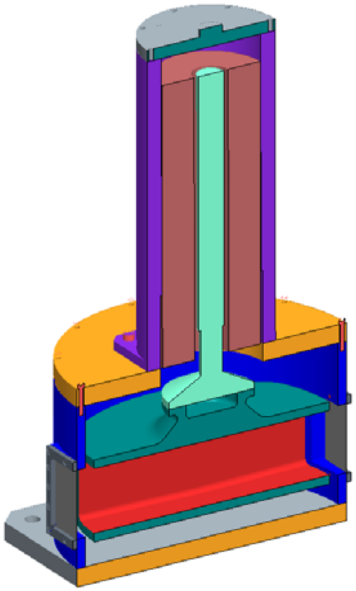




HOPG

Heusler

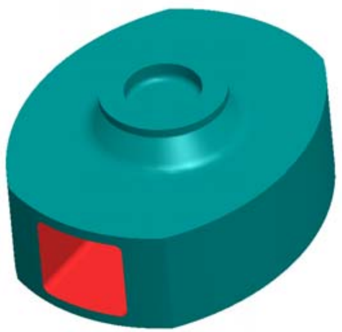
T0 Choppers and Curved Guides



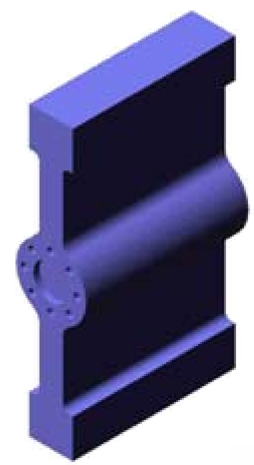
- When the proton beam strikes the target (time T0) a burst of ~1GeV neutrons and a flash of gamma rays are produced. Some are neutrons are moderated but some emerge into the beamline at time T0. Have to get rid of the fast neutrons and gamma rays.

- Two methods - T0 chopper or curved guide

- T0 chopper – rotating plug of Inconel (200 → 300mm) that blocks the beam at time T0. ARCS, SEQUOIA and HYSPEC have vertical axis version and VISION has horizontal axis version.



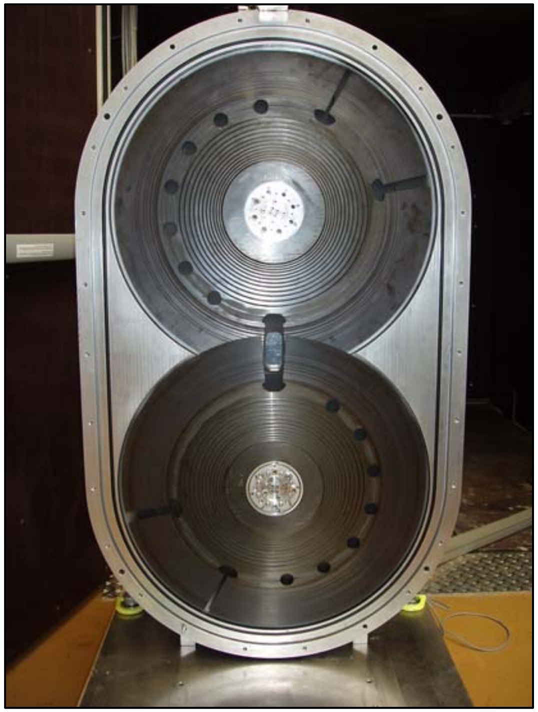
- Curved guide, low energy neutrons are reflected but not higher energies. The guide is curved so that final sample position does not have a line of sight to the source and fast neutrons must collide/be absorbed in, shielding around beamline. BASIS, CNCS and HYSPEC have curved guides.

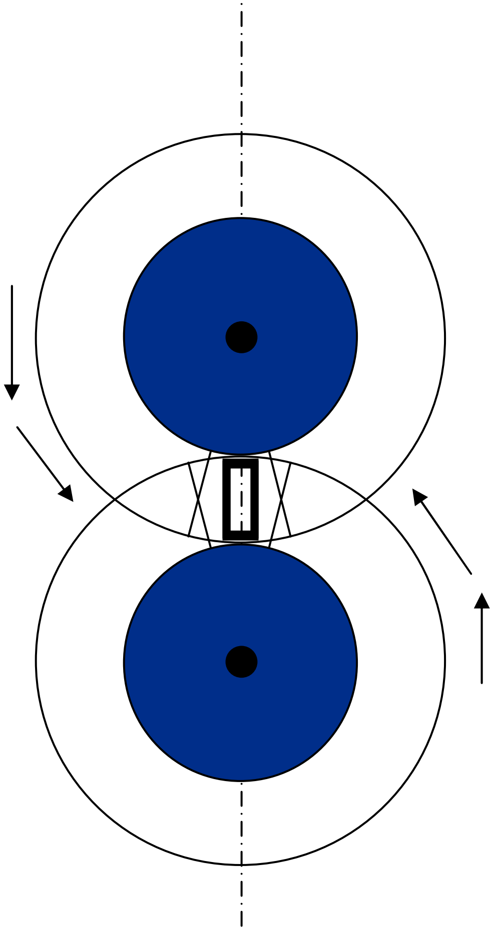


- Note T0 choppers are phased (electronically) to the source “T0” signal.

High Speed Double Disk Choppers - CNCS

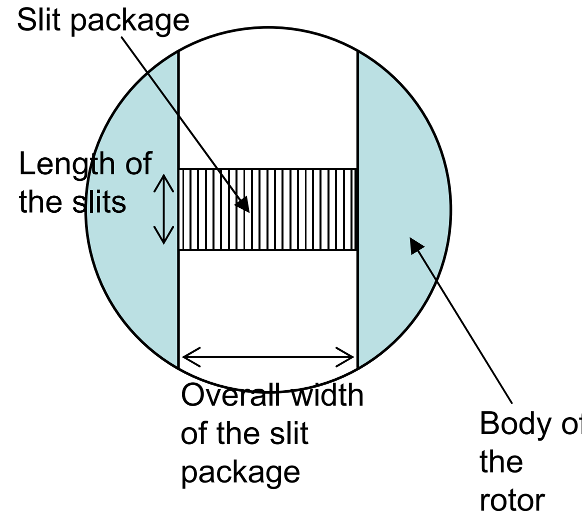
- In order to get high final energy resolution we need a short burst time for the chopper.
- If the 2 disks are rotating at 300Hz each then the effective frequency of the 2 choppers is 600Hz is this “counter-rotating” mode.
- Opening time is phased to T0 signal.

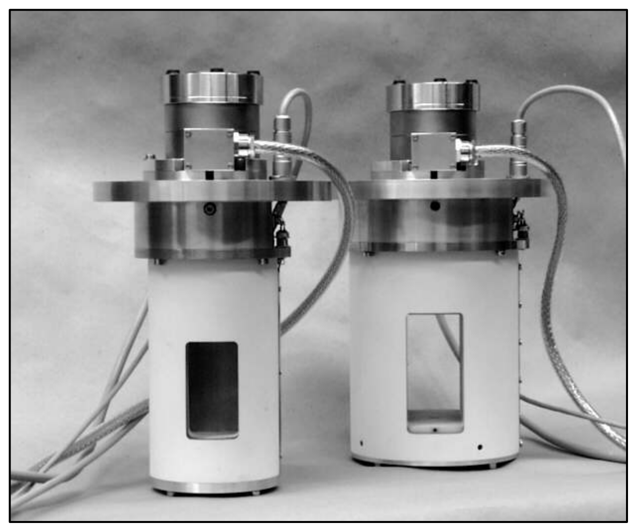


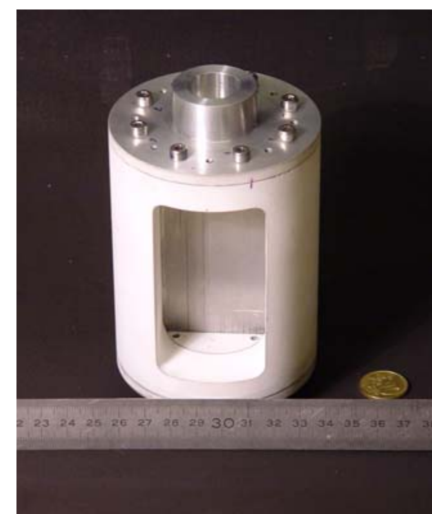


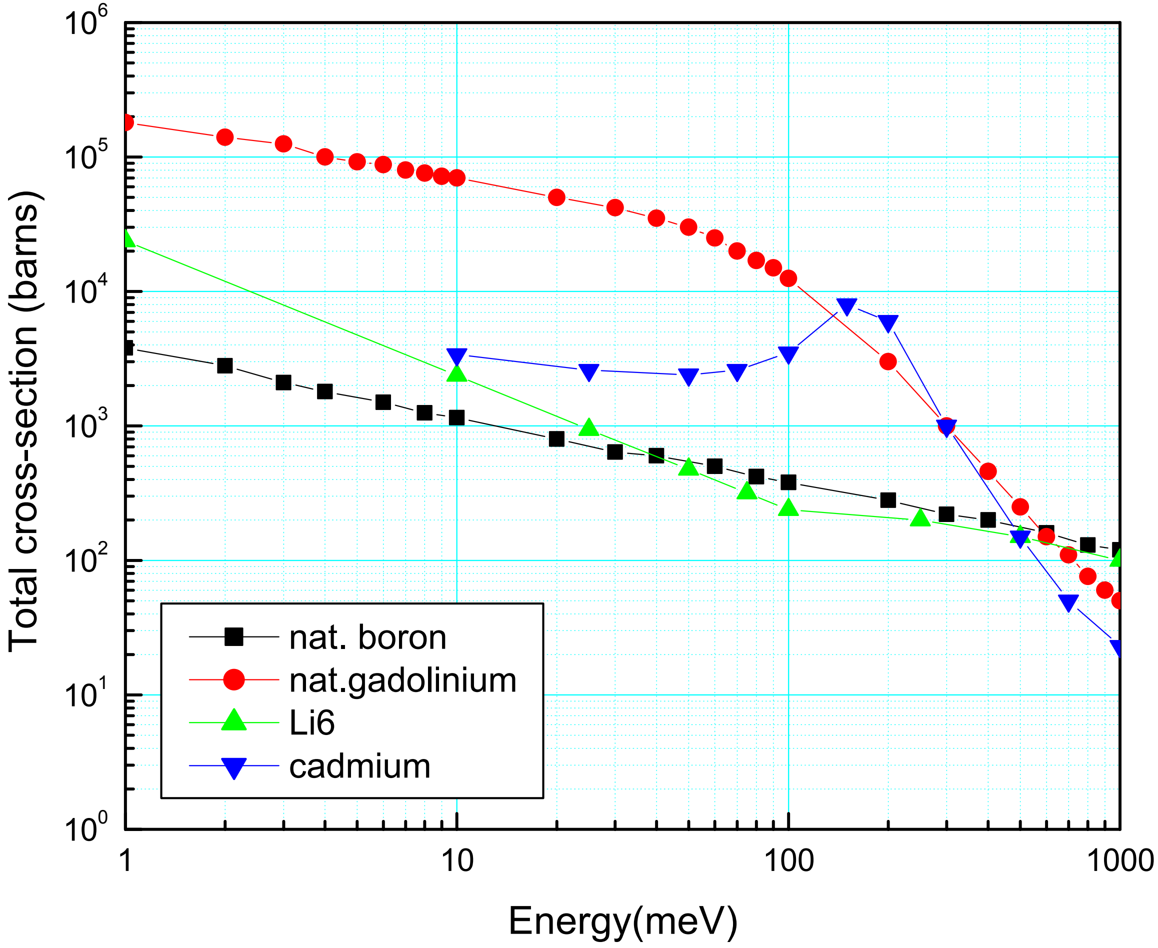
Fermi Choppers – ARCS, SEQUOIA, HYSPEC

- Rotating cylinders containing "slit" packages.
- Parallel to beam slits are "open" and close as cylinder rotates
- For ARCS/SEQUOIA long curved Al/B slit package
- For HYSPEC short straight Al/Gd slit package
- Open time for slit package is phased to T0
- Frequency 60Hz → 600Hz









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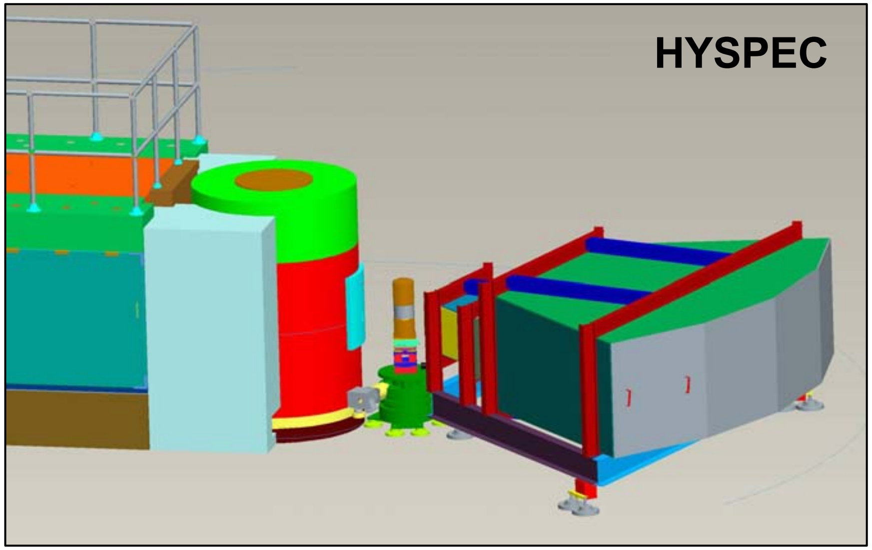
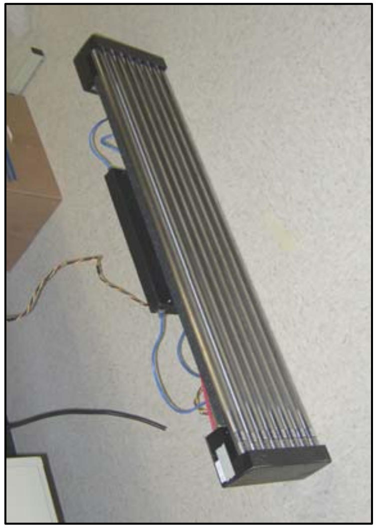
Detector Vessels: vacuum tanks – ARCS & SEQUOIA

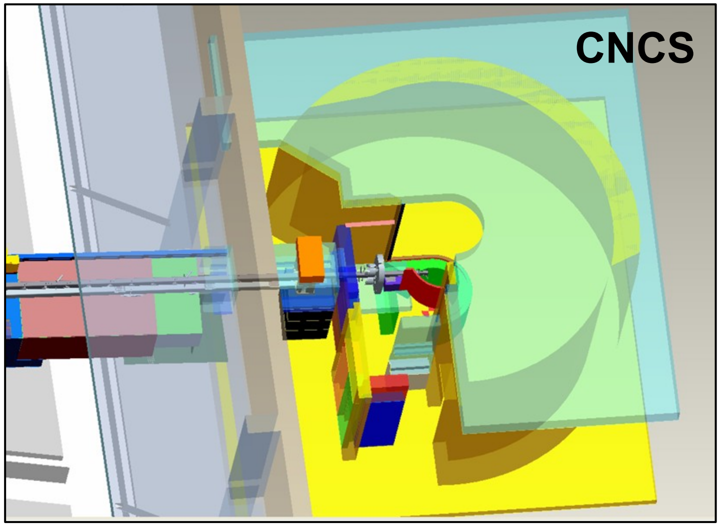
- Air scatters neutrons strongly, over long flight paths want to remove the air → vacuum
- Wallpaper the detector vessel with LPSD tubes

Detector vessels: Argon tanks – CNCS & HYSPEC

- If a vacuum tank isn't practical then an alternative is to use a tank or Argon.
- Ar has low scattering cross-section for n.
- Because Ar is at 1atm, windows can be thin Al and so very low scattering
- Again back of detector vessel is covered with LPSD's







Data: LPSD’s, DAS and NeXus translation

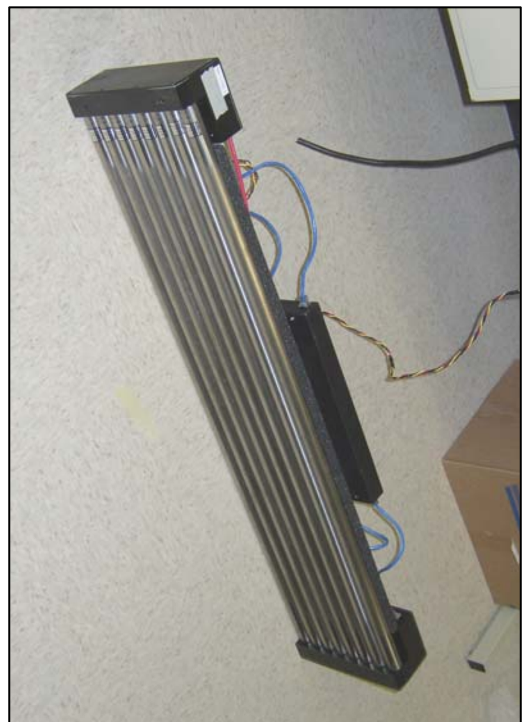
- LPSD = Linear Position Sensitive Detector (tube). A neutron absorption event in the ^{3}He gas in the tube causes electrical signals in the HV wire to travel to both ends of the tube. Difference in arrival time → position on tube, calculated by electronics on back of tube.

- DAS = Data Acquisition System. Receives T0 signal and broadcasts time on fibre optic network to electronics on back of 8 packs. When event occurs electronics on LPSD creates a word with position-id from LPSD and time-stamp from DAS clock and sends that off onto fibre optic network.

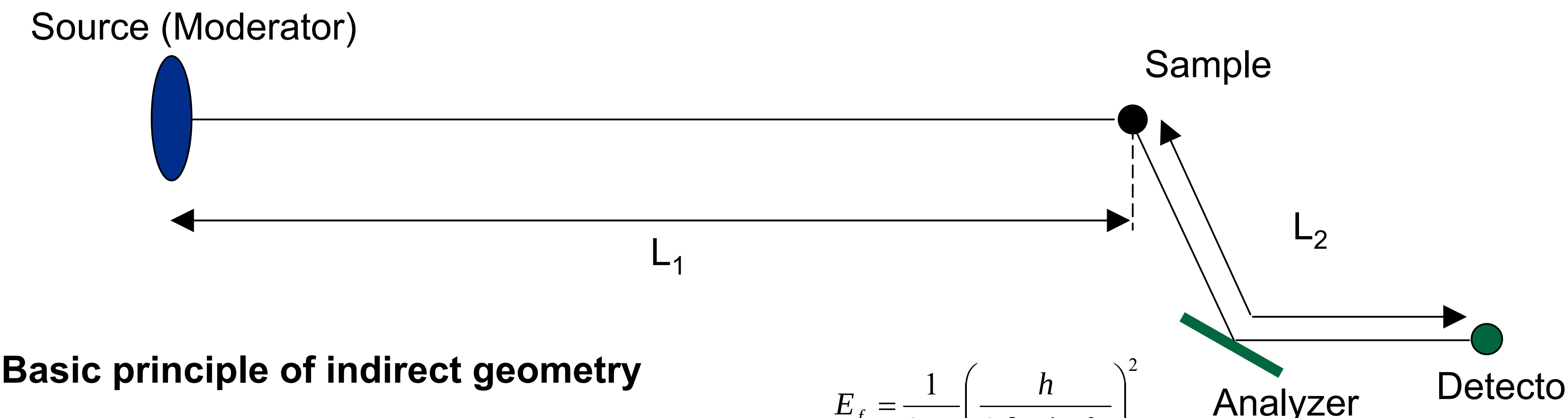
- DAS receives words/events from LPSD 8-packs and heaps them in a file.

- At end of run DAS downloads file to fileserver (along with monitor file).

- On fileserver software histograms the heap and creates a NeXus hierarchical data format (self describing) file for data reduction.



INDIRECT GEOMETRY



Basic principle of indirect geometry

- Indirect geometry = fixed final energy E_f
- Analyzer crystal defines the final energy via Bragg's law
- Because detected neutrons have a known energy, calculate and subtract final flight time after sample
- Hence obtain the incident flight time and E_i and consequently $E = E_i - E_f$

$$E_f = \frac{1}{2m_n}\left(\frac{h}{2d_A \sin\theta_A}\right)^2$$

$$T_{detector} = T0(E_i) + L_1\sqrt{m_n/2E_i} + L_2\sqrt{m_n/2E_f}$$

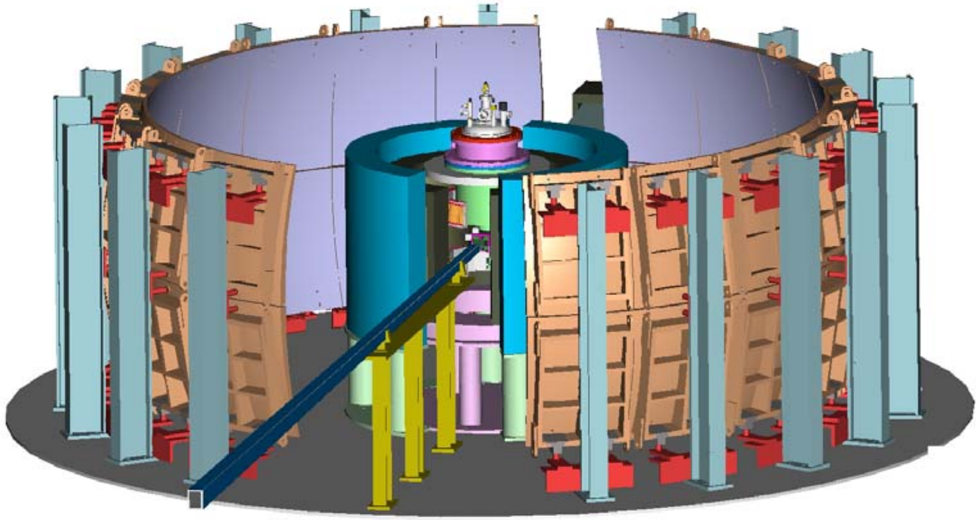
$$E_i = \frac{1}{2}m_n\left(\frac{L_1}{T_{detector} - T0(E_i) - L_2\sqrt{m_n/2E_f}}\right)^2$$

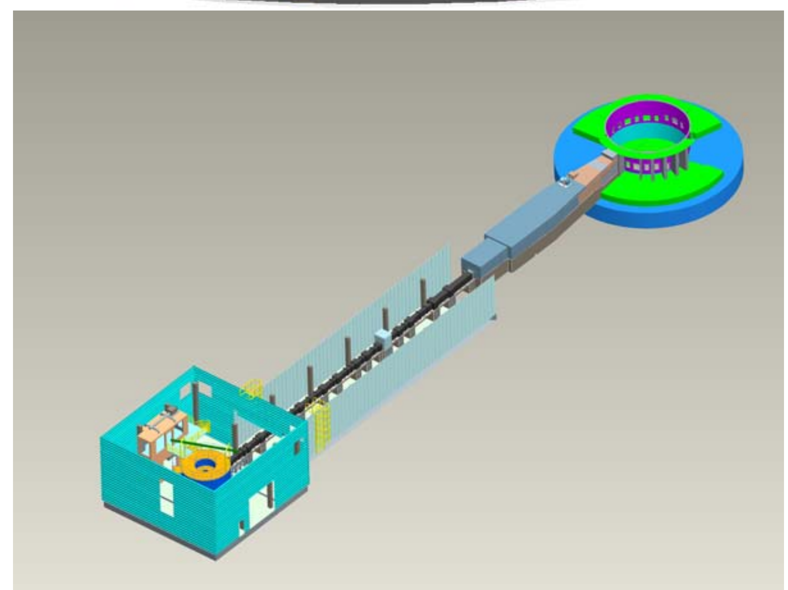
$$E = E_i - E_f$$

$$= \frac{1}{2}m_n\left(\frac{L_1}{T_{detector} - T0(E_i) - L_2\sqrt{m_n/2E_f}}\right)^2 - E_f$$

BASIS – backscattering spectrometer

- Source/Moderator
  - Decoupled supercritical Hydrogen, centerline poisoned
- Incident Flight Path - 84 m moderator-sample position
  - Curved Guide: 10 cm wide x 12 cm tall, 1000 m radius of curvature, line-of-sight at 31 m
  - Straight Guide: 10 cm wide x 12 cm tall
  - Converging Funnel exit: 3.25 cm x 3.25 cm, stops 27.5 cm from sample
- Chopper System - 3 bandwidth/frame overlap choppers
- Sample – nominal dimensions 3 x 3 cm^2
- Radial Collimator – restricts analyzer view of the sample, Final Flight Path - 2.5 m sample - analyzer, ~ 2 m analyzer – detector
- Detector Choice – ^3He LPSD tubes, peak count rate (elastic, 30% scatterer) 4000 counts/cm2 /sec
- Analyzer Crystals
  Si (111): λ_f = 6.267 Å, $\delta d/d \sim 3.5 \times 10^{-4}$, 2.03 ster, 12.5 m^2, bandwidth 0.785 Å



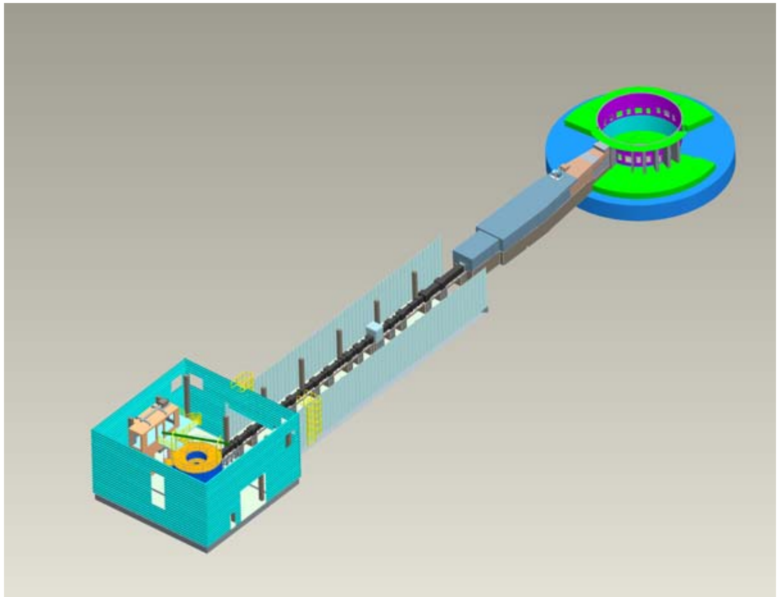


Why Backscattering & long flight path?

- Want high resolution, BASIS has ΔE = 3.5ueV
- So need high resolution for both ΔE_f and ΔE_i since $E = E_i - E_f$.
- For E_f look at Bragg's law results Cot $\theta_A \rightarrow 0$ for $\theta_A \rightarrow 90°$ i.e. $2\theta_A \rightarrow 180°$
- On BASIS the Bragg angle is $\theta_A \sim 88°$
- We obtain E_I by time of flight over a distance. If we want very accurate ΔE_i we need to time over a very long distance.
- On BASIS L_1 is 84m.

$$E_f = \frac{1}{2m_n}\left(\frac{h}{2d_A \sin\theta_A}\right)^2$$

$$\frac{\Delta E_f}{E_f} = -2\cot\theta_A \Delta\theta_A$$



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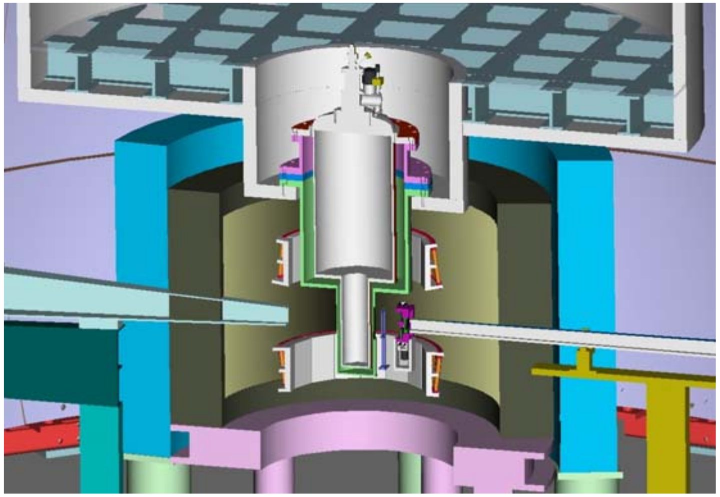
SPACKLE SING SNS



- Neutrons are backscattered from the spherical analyzers into the pixels on the LPSD's

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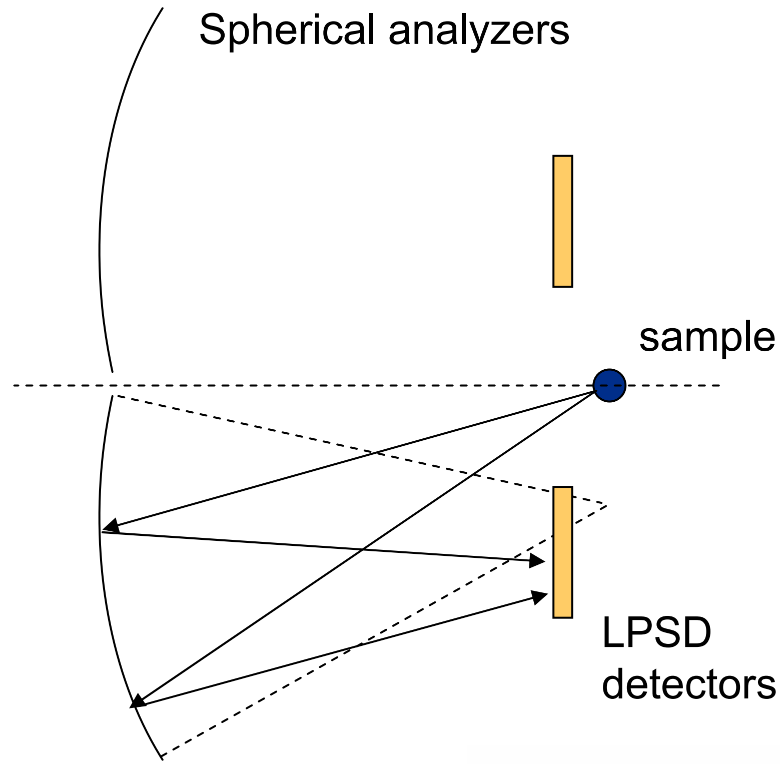
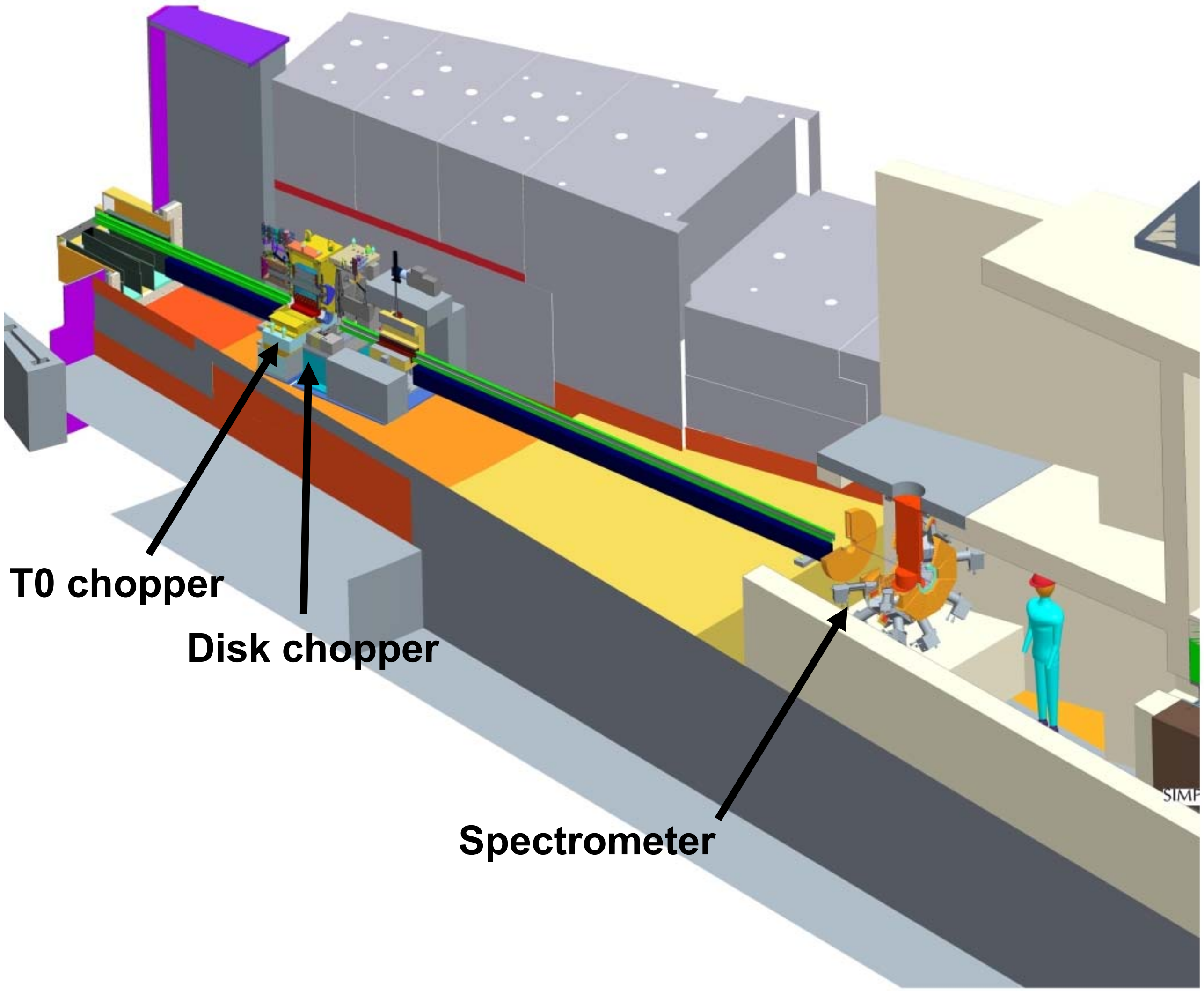
- Because spherical reflection angles (and hence also E_f's) differ pixel to pixel

.

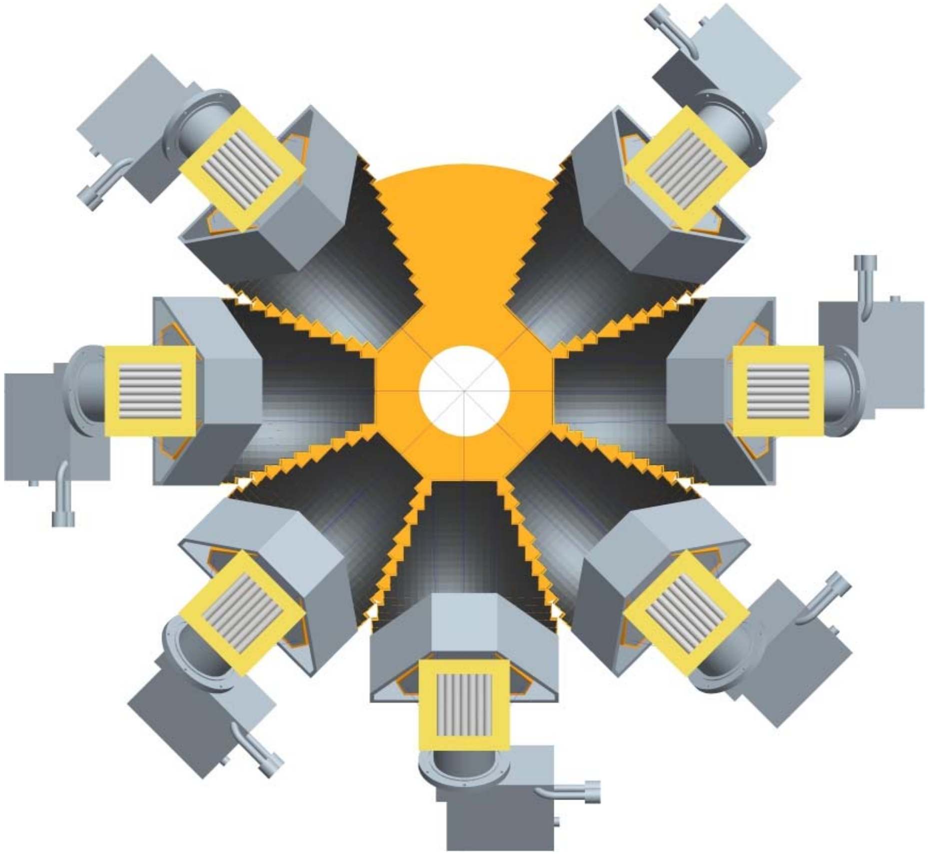
- Need to do the indirect geometry ToF to energy transfer on a pixel to pixel basis.



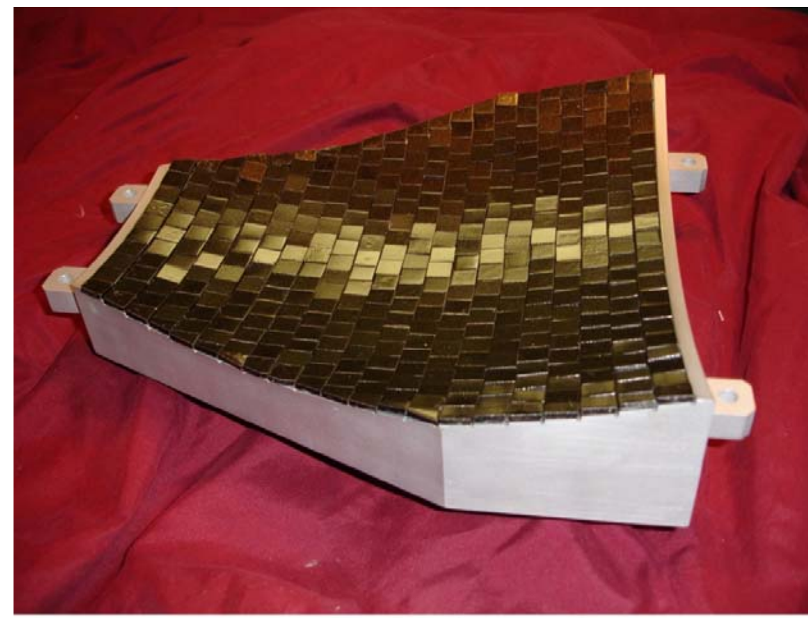
VISION – chemical spectroscopy



- For molecular excitations over wide energy range E_i goes up to ~500meV
- Short beam line for high intensity
- Indirect geometry with 14 analyzer panels covered HOPG crystals
- HOPG = Highly Oriented Pyrolitic Graphite



- Neutrons reflect off HOPG crystals on spherical surface into LPSD tubes
- For (002) reflections of HOPG analyzing energy is ~4meV
- Again do pixel by pixel transformation from ToF energy transfer



- Need Be filters to reject neutrons scattered by (004) and (006) planes in HOPG. Roughly Be transmits neutrons for E_f < 5meV and scatters for E_f > 5meV.

- VISION also uses time focusing on the analyzers to improve the energy resolution

Summary/Close-out

- Very brief "how it works" review of the SNS spectrometers

  Direct geometry – ARCS, SEQUOIA, CNCS and HYSPEC
  Indirect geometry – BASIS and VISION

- Haven't touched on

  Background (from cryostats/holders etc.) reduction in hardware
  Data reduction:
    Background subtraction in software
    Jacobians – we measure in pixels & ToF but want S(Q,E)
    Normalization of spectra by monitor for BASIS & VISION
    Detector efficiency normalization
  Data Analysis when we get to S(Q,E)

- These would all be 1 hour long "tutorials", hopefully this one is a "good start"