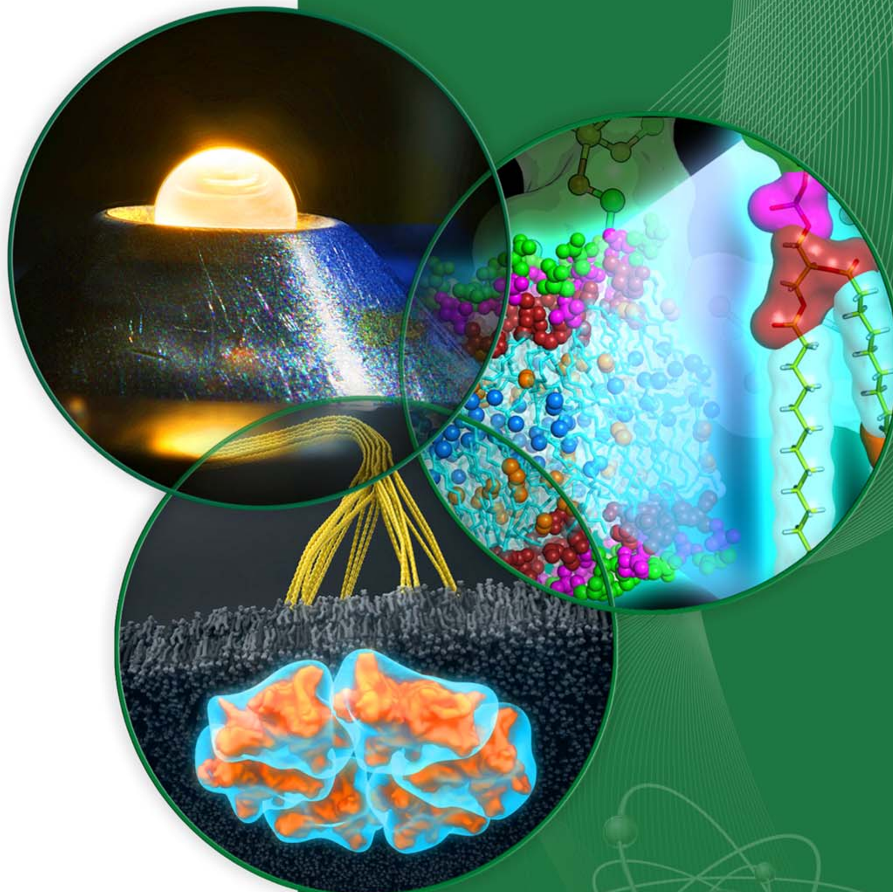
Design Considerations for Time-of-Flight Instruments

SNS Second Target Station



Presented to
2016 Neutron Lifecycle Lecture Series

Presented by
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Oak Ridge National Laboratory

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Outline

- Instrument Design: Where do you start?
- Time-of-flight Resolution (wavelength and energy) and Flux
  - A simple powder diffractometer
  - Flight paths/moderators/choppers
  - Short-pulse or Long-pulse source
- Moderator Characteristics and Instruments
- An Inelastic Example
  - Inverse Geometry on short-pulse source (long-pulse)
- Background and Signal-to-Noise
- SNS Second Target Station – a brief overview
- Where do all the neutrons go?

Instrument Design -Some General Observations

- The ultimate goal is not to build an instrument but to build a tool to deliver science
- Complementarity to other instruments may be important – understand the relationship of your beam line to others (and other characterization techniques)
- Your design should leverage modern advances in neutron hardware and techniques
- Be wary of complexity – the instrument has to work in the real world not just on paper (or in the computer)
- Pay attention to the details
  - Beam line windows
  - Operational considerations – reliability/maintainability/access
- Don't be afraid to seek advice
- You must finish – designing and building an instrument is not an open-ended research project

Where do you start?

- Define the science capability you are tasked to deliver, then translate that into performance requirements for the instrument
  - Energy and wavelength resolution
  - Q-resolution
  - Highest count rate or Highest resolution – what are your optimization parameters?
- Understand your source characteristics
  - Neutron Spectra – cold source/moderator, ambient temperature …
  - Time structure
  - Available geometry
- With a calculator, pencil and paper (or maybe a spreadsheet) – you can often go a long way in an instrument design on the "back of an envelope" and with approximations

Science Capabilities

- What do you want to learn?
  - Powder diffraction, single x-tal diffraction, SANS, inelastic, reflectometry
- What form is the sample?
  - Powder, liquid, crystalline, glass, surface
  - Size
- What types of sample environment do you need to accommodate?
  - Cryogenic, furnace, high-pressure, magnetic fields, humidity, electric field

Time-of-Flight – Energy and Wavelength Resolution

$$\lambda = \frac{3956}{v}; \quad \lambda(\text{Å}),\ v\left(\frac{\text{m}}{\text{s}}\right)$$

$$= 3956\,\frac{t}{L};\ t(\text{s}),\ L(\text{m})$$

$$\delta\lambda = 3956\left[\frac{(\delta t)^2}{L^2} + \frac{t^2}{L^4}(\delta L)^2\right]^{1/2}; \qquad \frac{\delta\lambda}{\lambda} = \left[\frac{(\delta t)^2}{t^2} + \frac{(\delta L)^2}{L^2}\right]^{1/2}$$

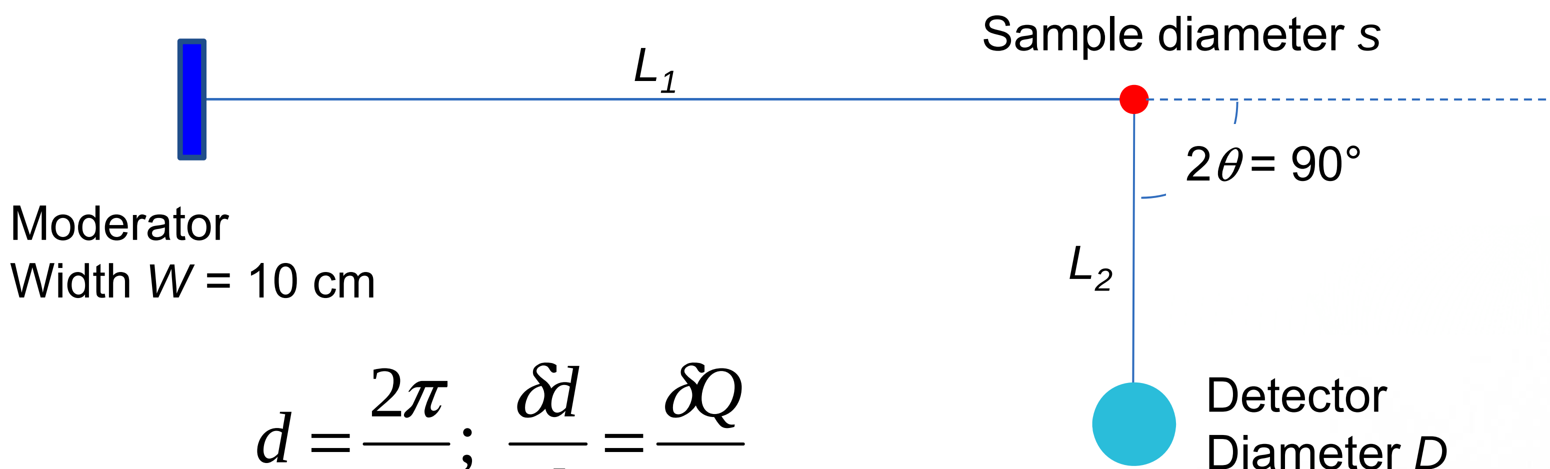
Assumes that *t* and *L* are independent and that contributions add in quadrature

$$E = \frac{81.8}{\lambda^2};\ E(\text{meV}); \quad E = 5.227\times10^{-6}\,\frac{L^2}{t^2}$$

$$\delta E = 2\,\frac{81.8}{\lambda^3}\,\delta\lambda; \quad \frac{\delta E}{E} = 2\,\frac{\delta\lambda}{\lambda}$$

Simple Powder Diffractometer

- Science Goals
  - Measure a *d*-spacing range at 90° of 0.2 Å to 4.0 Å
  - With a resolution $\delta d/d$ at 90° less than or equal to 1×10^{-3}
  - And a maximum sample size of 6 mm diameter, 30 mm tall



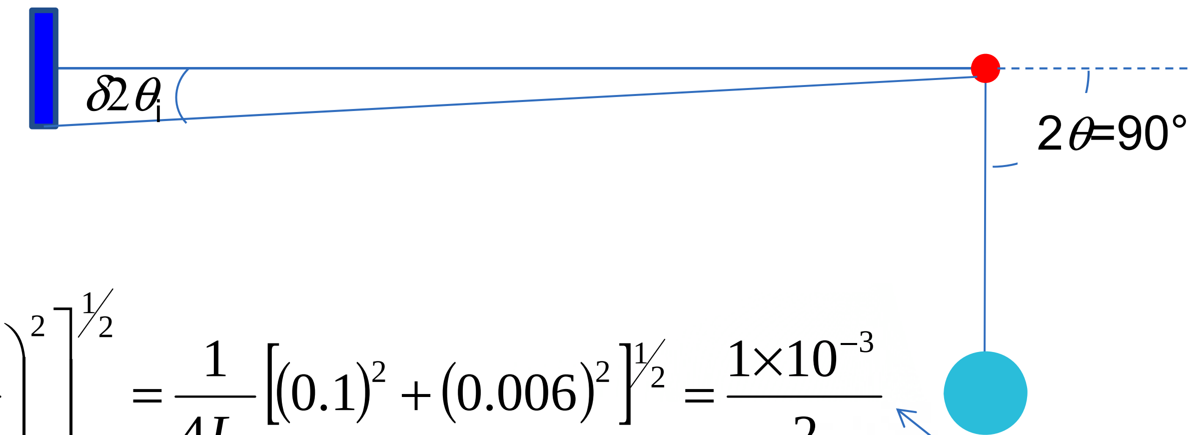
$$d = \frac{2\pi}{Q}; \quad \frac{\delta d}{d} = \frac{\delta Q}{Q}$$

$$Q = \frac{4\pi \sin(\theta)}{\lambda}; \quad \frac{\delta Q}{Q} = \left[\frac{(\delta\lambda)^2}{\lambda^2} + \cot^2(\theta)(\delta\theta)^2 \right]^{1/2}$$

Q-resolution – geometrical contribution

Requirement is that $\dfrac{\delta Q}{Q} = 1\times 10^{-3}$

We will choose to match the two contributions to the Q-resolution [cot(45) = 1] $\dfrac{\delta\lambda}{\lambda} = \cot(\theta)\delta\theta = \delta\theta = \dfrac{1\times 10^{-3}}{\sqrt{2}}$



$$\delta\theta = \left[(\delta\theta_i)^2 + (\delta\theta_f)^2\right]^{1/2}$$

$$\delta\theta_i = \frac{1}{2}\delta 2\theta_i \approx \frac{1}{2}\left[\left(\frac{W}{2L_1}\right)^2 + \left(\frac{s}{2L_1}\right)^2\right]^{1/2} = \frac{1}{4L_1}\left[(0.1)^2 + (0.006)^2\right]^{1/2} = \frac{1\times 10^{-3}}{2}$$

Taking $\delta\theta_i$ = $\delta\theta_f$

$$\delta\theta_f \approx \frac{1}{2}\left[\left(\frac{D}{2L_2}\right)^2 + \left(\frac{s}{2L_2}\right)^2\right]^{1/2} = \frac{1}{4L_2}\left[(0.006)^2 + (0.006)^2\right]^{1/2} = \frac{1\times 10^{-3}}{2}$$

Matching detector and sample dimension

$L_1 \geq 50$ m $\quad$ $L_2 \geq 4.24$ m

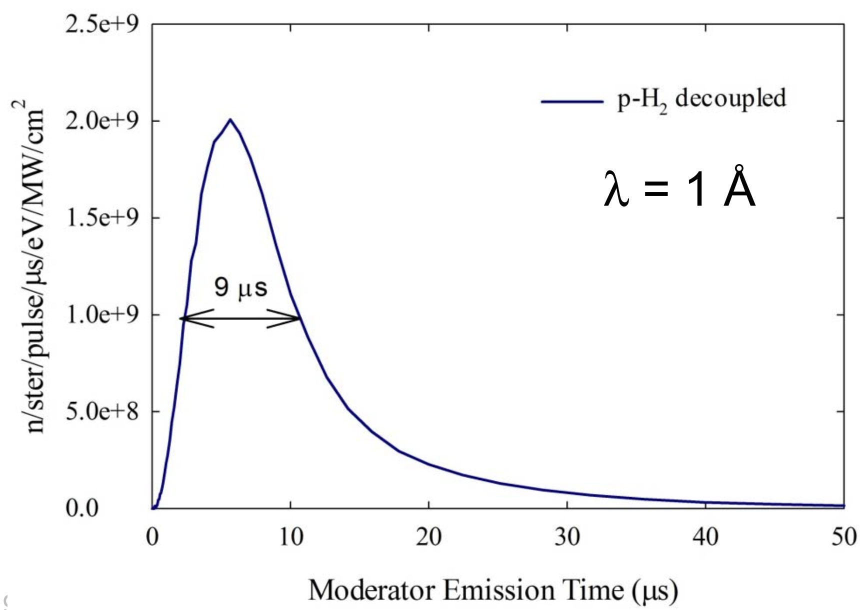
Q-resolution – wavelength contribution

$$t = \frac{\lambda(L_1 + L_2)}{3956} = \frac{\lambda L}{3956}$$

Estimate effect of finite sample size; the neutron could scatter from any point in the sample

$$\frac{\delta\lambda}{\lambda} = \left[\frac{(\delta t)^2}{t^2} + \frac{(\delta L)^2}{L^2}\right]^{1/2} = \left[\frac{(\delta t_{\mathrm{mod}})^2}{(\lambda L)^2 / 3956^2} + \frac{0.006^2}{L^2}\right]^{1/2}$$

For L = 54.24 m, we would like $\delta t_{\mathrm{mod}} \approx$ 9.6 x 10^{-6} s at λ = 1 Å



For this moderator type,

$\delta t_{\mathrm{mod}} \approx$ 9 x 10^{-6} λ s

Which means that this moderator will satisfy our requirements at all relevant wavelengths

Why not make the final flight path (L_2) longer?

- The resolution improves and/or the sample could be larger
- There is no impact on the number of scattered neutrons
- The detector spatial resolution requirements are easier to achieve

COST

To cover the same solid angle (intercept the same number of scattered neutrons) costs quadratically in terms of amount of detector coverage. Size of the scattering vessel increases and shielding around detectors gets bigger and also costs more.

COST is one of the parameters that goes into instrument optimization and design!

Repetition Rate and Frame Overlap

- Requirement is d_{min} = 0.2 Å and d_{max} = 4 Å at a Bragg angle of 45°.

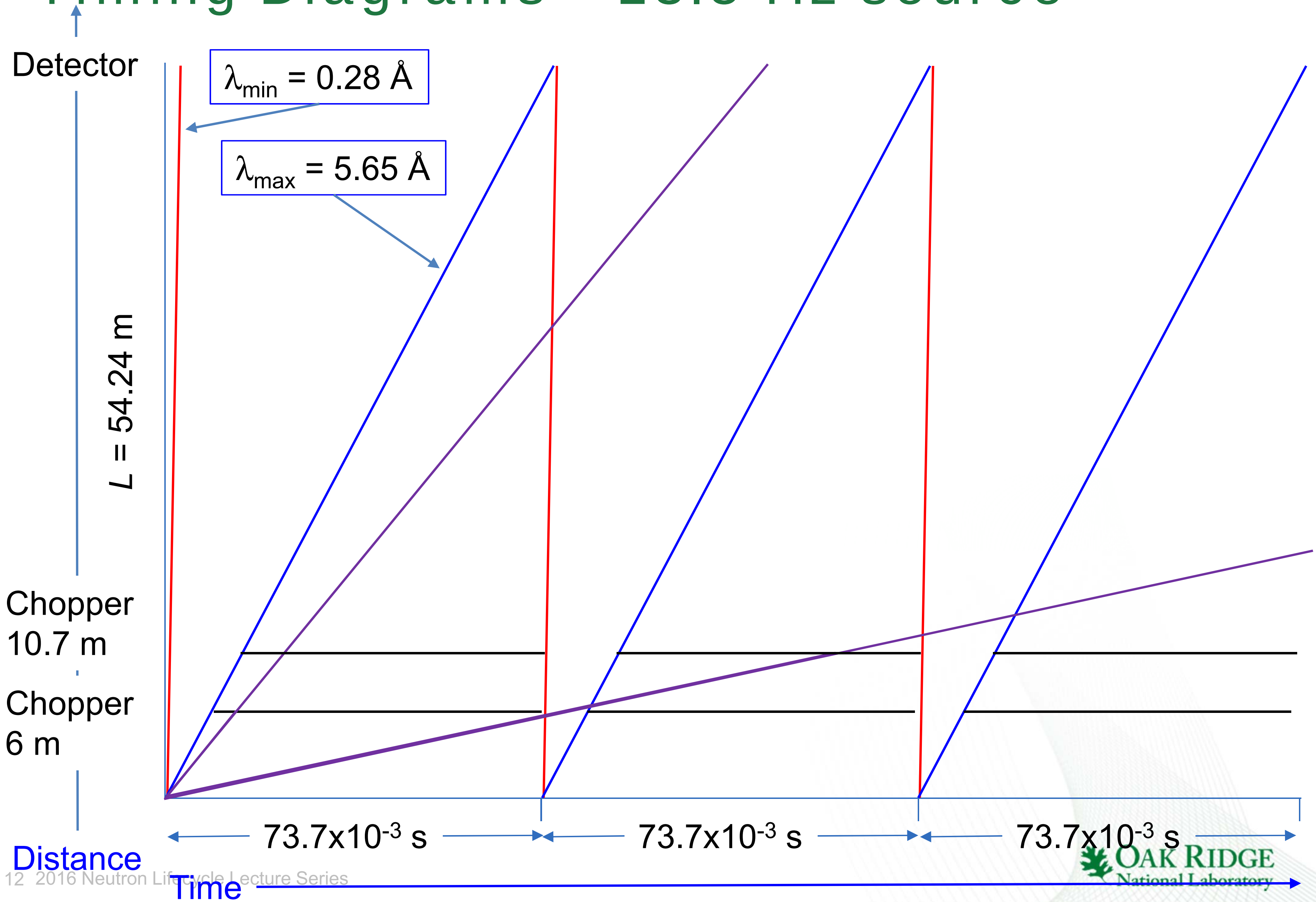
$$d = \frac{\lambda}{2\sin(\theta)} = \frac{\lambda}{1.414} \text{ at } \theta = 45°$$

$$d_{max} - d_{min} = \frac{\lambda_{max} - \lambda_{min}}{1.414} = \frac{\Delta\lambda}{1.414};\ \ \Delta\lambda = 5.37\,\text{Å}$$

$$\Delta t = \frac{L\Delta\lambda}{3956} = \frac{54.24 \times 5.37}{3956} = 0.0737\text{s}$$

- Desired source frequency is $1/\Delta t$ = 13.6 Hz
- SNS is a 60 Hz facility, what are my options
  - Suppress 3 out of 4 frames and operate at effective 15 Hz
  - Add detectors at additional scattering angles
  - Shift the wavelength band and make 4 – 5 sequential measurements taking 4 – 5 times longer count times

Timing Diagrams – 13.5 Hz source



What if I have a long-pulse source?

- ESS will have an intrinsic pulse width of 2.86 x 10^{-3} s and will operate at 14 Hz (nearly the same as our example).
  - To use this pulse width and get the same wavelength resolution as our example would require an instrument length of

$$\frac{\delta\lambda}{\lambda} = \frac{1\times10^{-3}}{\sqrt{2}} \approx \frac{\delta t_{\mathrm{mod}}}{(\lambda L)/3956}$$

$$L = \frac{\sqrt{2}}{1\times10^{-3}} \times \frac{\delta t_{\mathrm{mod}}}{\lambda/3956} = 16,000\ \mathrm{m}$$

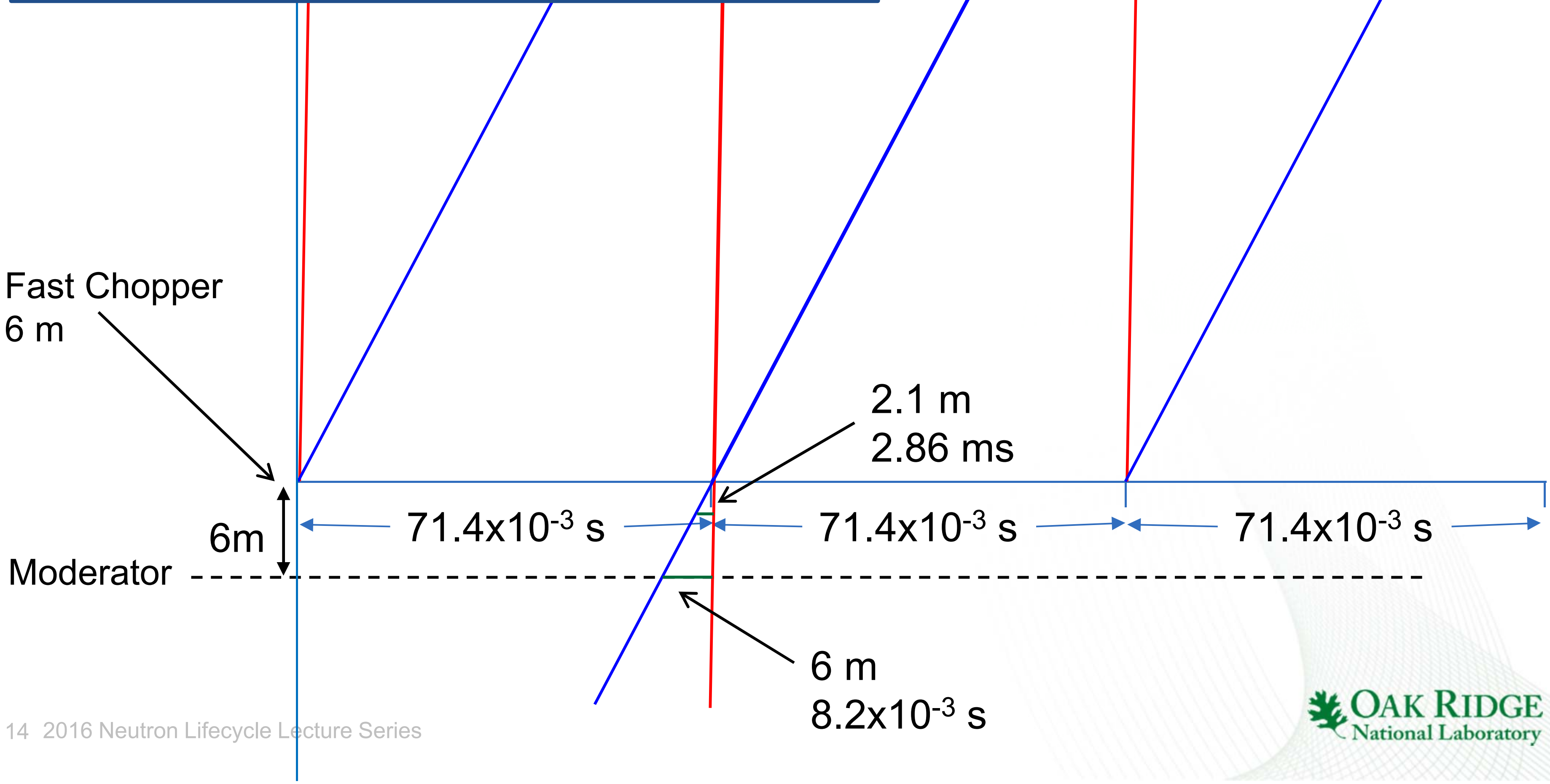
  - You must create sharper bursts of neutrons using a fast chopper!

Fast Chopper and bandwidth

You would like a pulse duration of

$$\Delta t = \frac{l_{chop}\Delta\lambda}{3956} = \frac{6\times 5.4}{3956} = 8.2\times 10^{-3}\,\text{s}$$

Or put the chopper only 2.1 m from moderator



What are my options?

- Make the instrument longer
  - Constant resolution means Fast chopper can be open longer
  - More neutrons (in a narrower wavelength band)
  - Longer instrument means smaller bandwidth
  - For a fast chopper at 6 m – bandwidth would be 1.9 Å, instrument length would be 149 m, Chopper open time to match resolution of example instrument would be 25×10^{-6} s (remember our optimal moderator pulse width for 54.24 m instrument was 9.6×10^{-6} s).
  - But - Neutron transport may be an issue!
- Keep the instrument the same length
  - Use more micro-pulses/primary pulse (repetition rate multiplication/wavelength frame multiplication)

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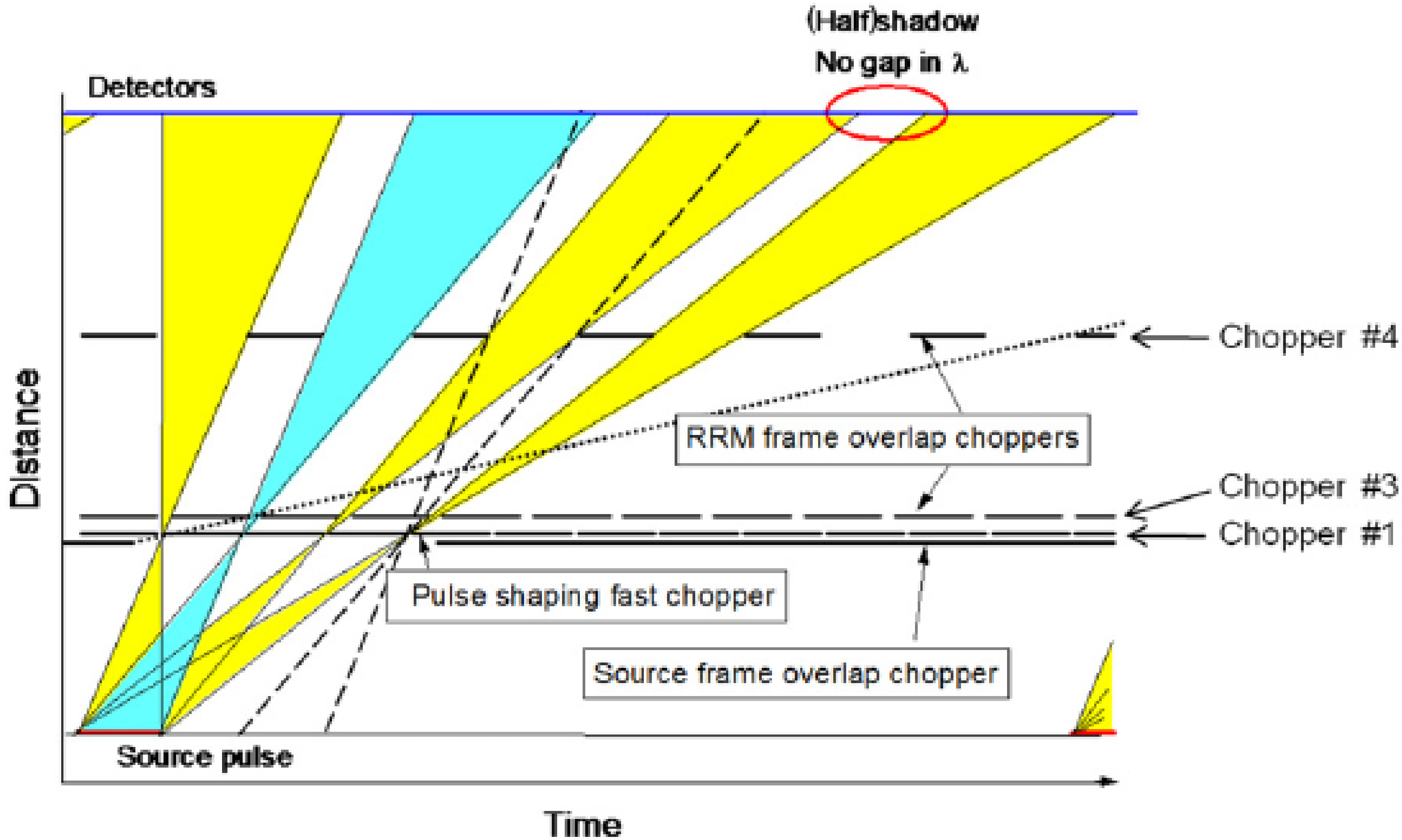
Illustration of Multiplexing Schemes



M. Russina, et al., Nucl. Instrum. Meth. A **654**, 383-389 (2011)

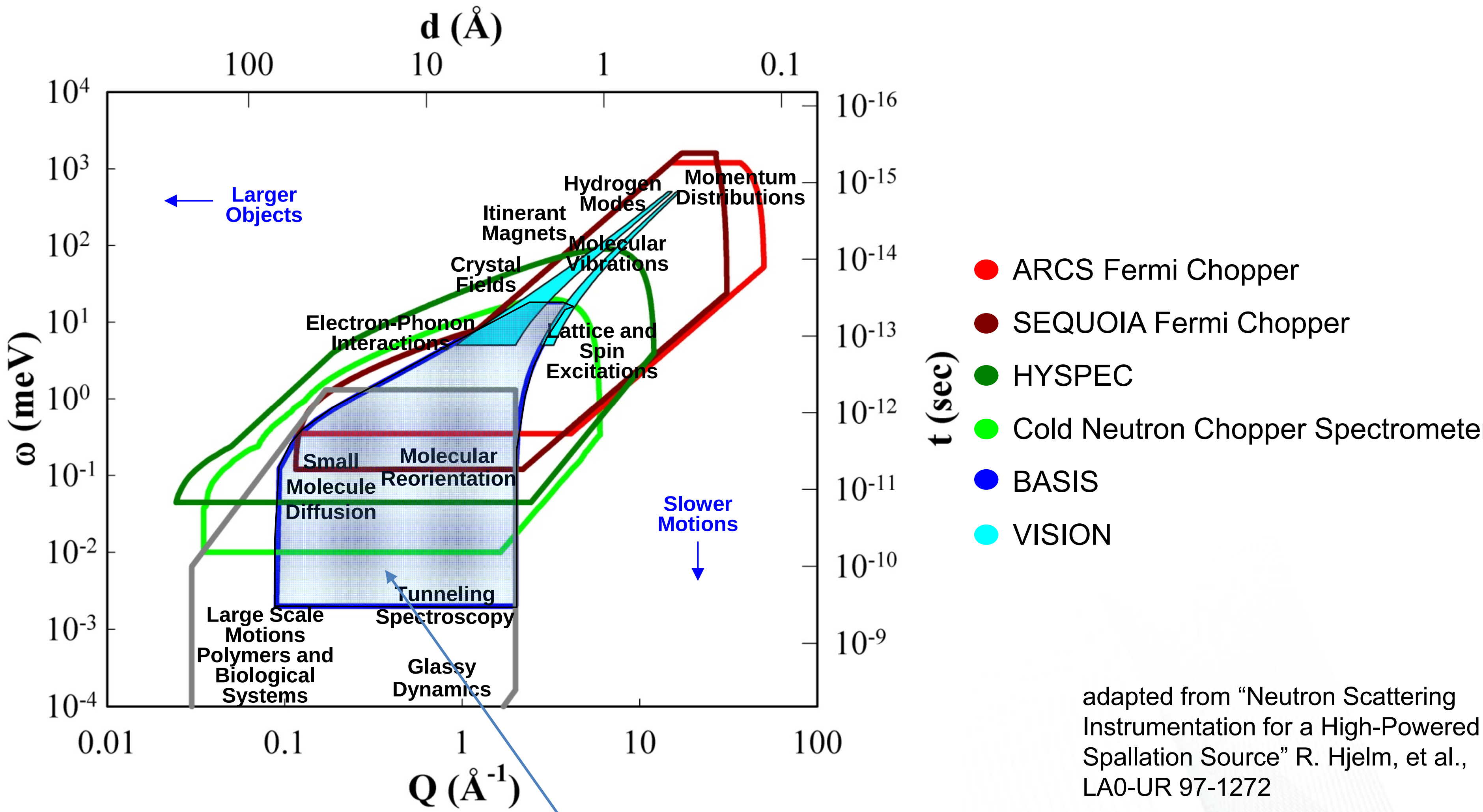
Instruments, Moderators and Source

- Moderators and Sources – 3 main characteristics
  - Neutron Intensity as a function of wavelength
  - Neutron Pulse Width as a function of wavelength
  - Repetition rate – source frequency – determines the usable wavelength band for a given length beam line
- 4 instrument categories
  - Performance driven largely by integrated flux on sample – SANS, Neutron Spin-Echo and Reflectometers(?)
  - Performance driven by high peak flux, narrow band width – Multi-chopper spectrometers
  - Performance driven by narrow pulse widths but need a large effective band width. High-resolution powder diffractometers and high resolution (backscattering) spectrometers.
  - Performance driven by sample size with reasonable pulse widths. High-pressure diffractometer and single-crystal diffractometer.

Spectrometers – Inelastic Scattering

- Time-of-flight only determines one of the two neutron energies, either the energy of the incident or the energy of the scattered neutron.
- Direct geometry spectrometers – monochromatic incident beam, scattered neutron energy determined by time-of-flight
  - Cold neutron chopper spectrometers and Fermi chopper spectrometers
  - Flexible
  - Very high signal-to-noise (low background)
- Indirect geometry spectrometers – scattered neutron energy is selected by analyzer crystals (Bragg scattering), incident neutron energy is determined by time-of-flight
  - Near backscattering spectrometers
  - Highest combination of energy resolution/flux/Q-range
  - Typically modest Q-resolution
  - Inelastic scattering – works in neutron energy loss

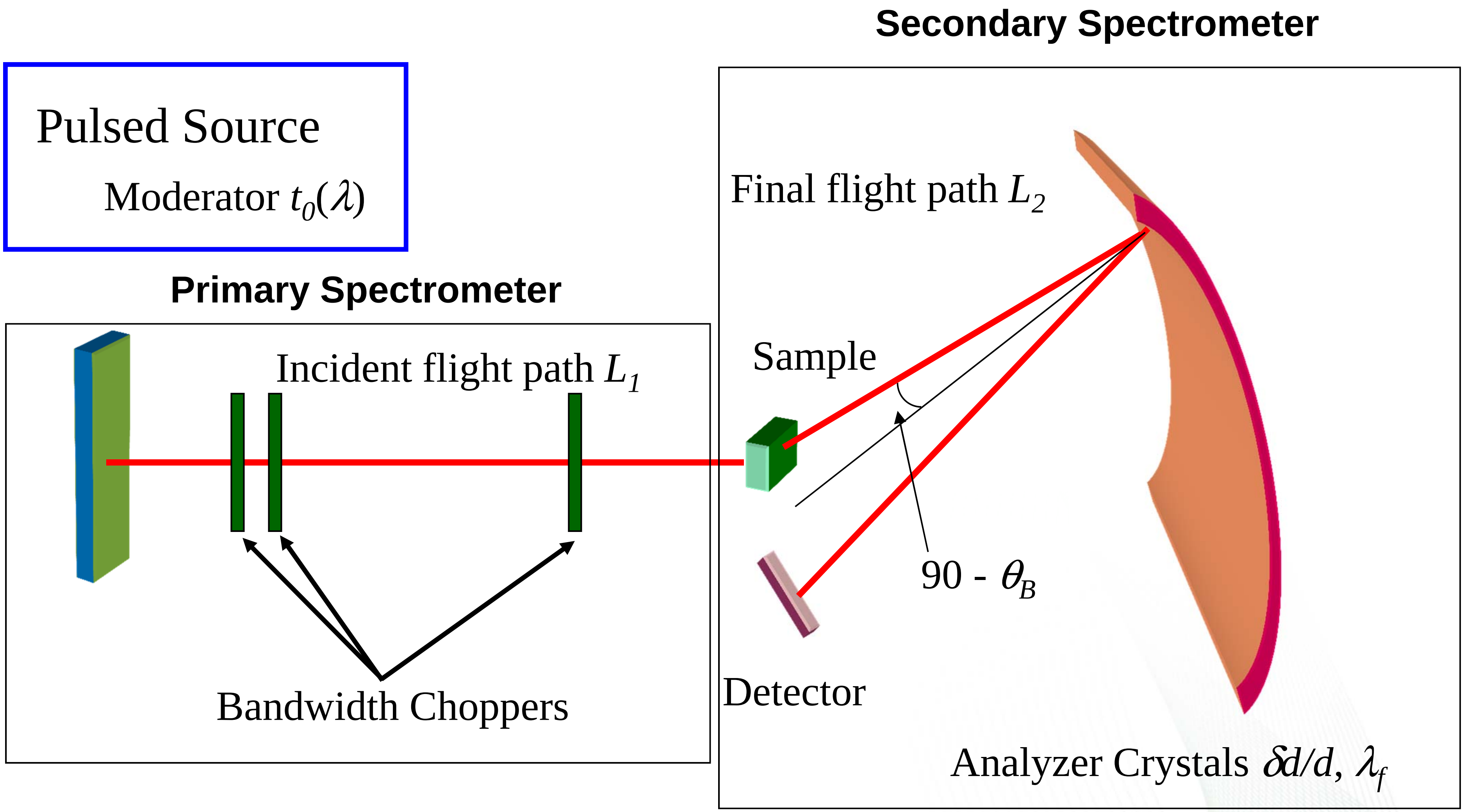
SNS Spectrometer Landscape



adapted from “Neutron Scattering Instrumentation for a High-Powered Spallation Source” R. Hjelm, et al., LA0-UR 97-1272

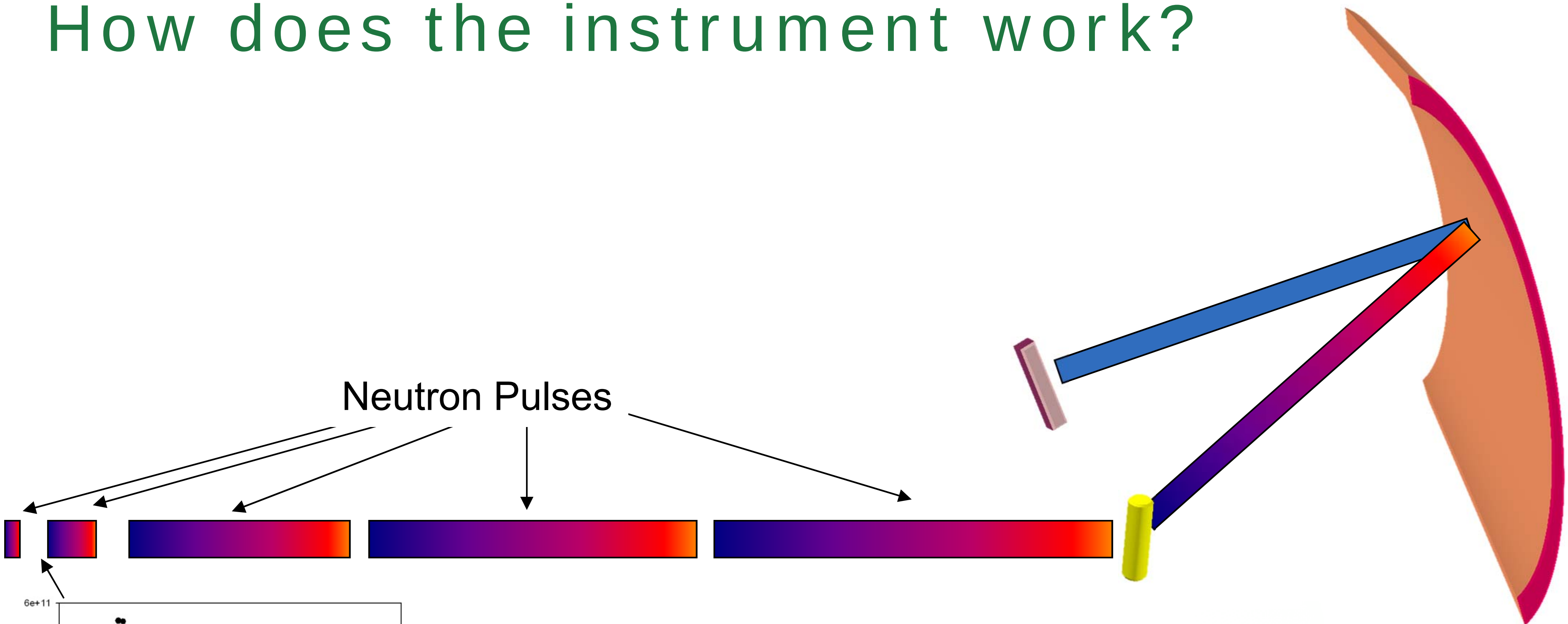
BaSiS – Indirect Geometry, Near-backscattering Spectrometer

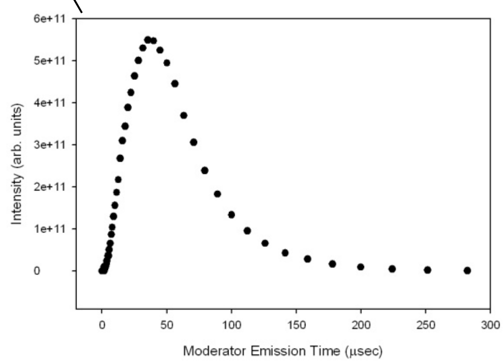
Crystal Analyzer Spectrometers and the Resolution Function



t_f = time for neutrons to travel from sample-analyzer-detector = $(L_2\lambda_f/3956)$

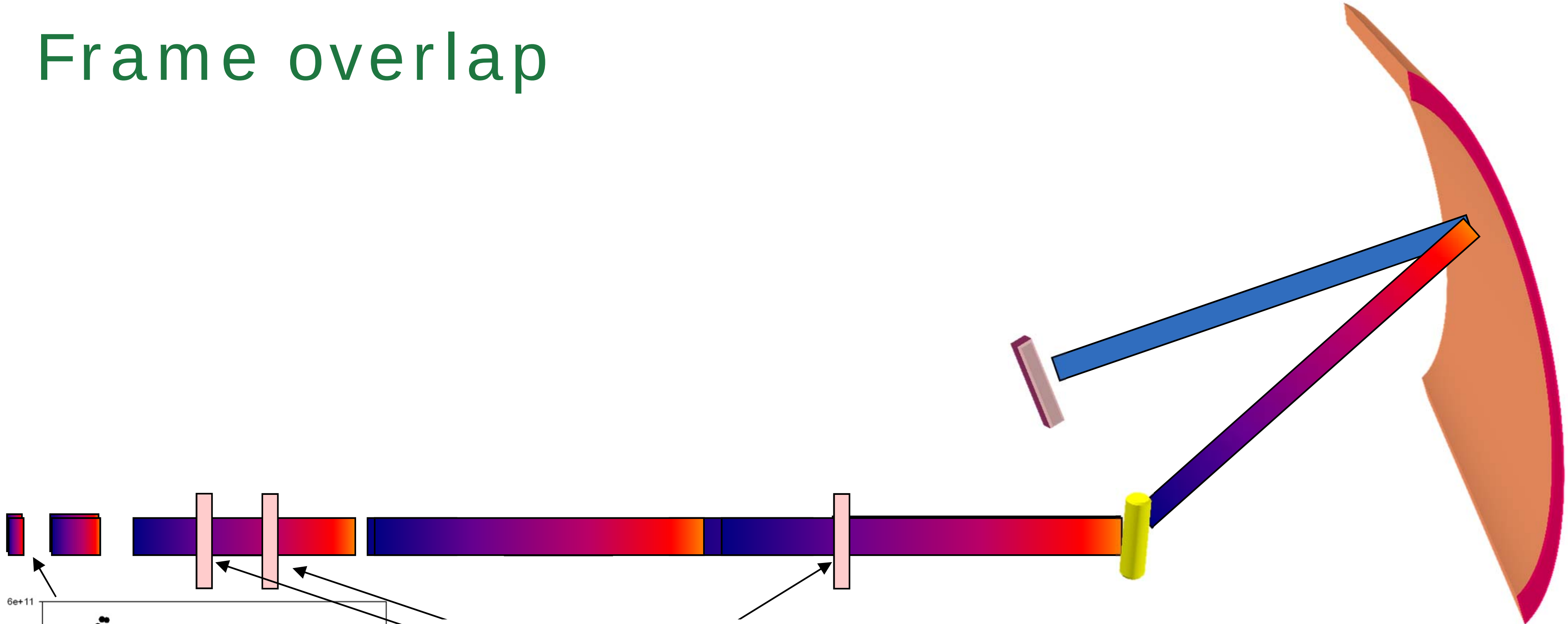
How does the instrument work?

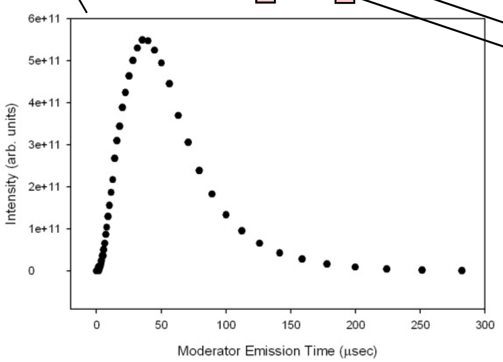




- Time-of-flight selects the incident neutron velocity
- Analyzer crystal selects the final neutron velocity
- At 84 m long, BaSiS has 9 “trains” of neutrons in the incident flight path at any given time (at 60 Hz)

Frame overlap





- Time-of-flight selects the incident neutron velocity
- Analyzer crystal selects the final neutron velocity
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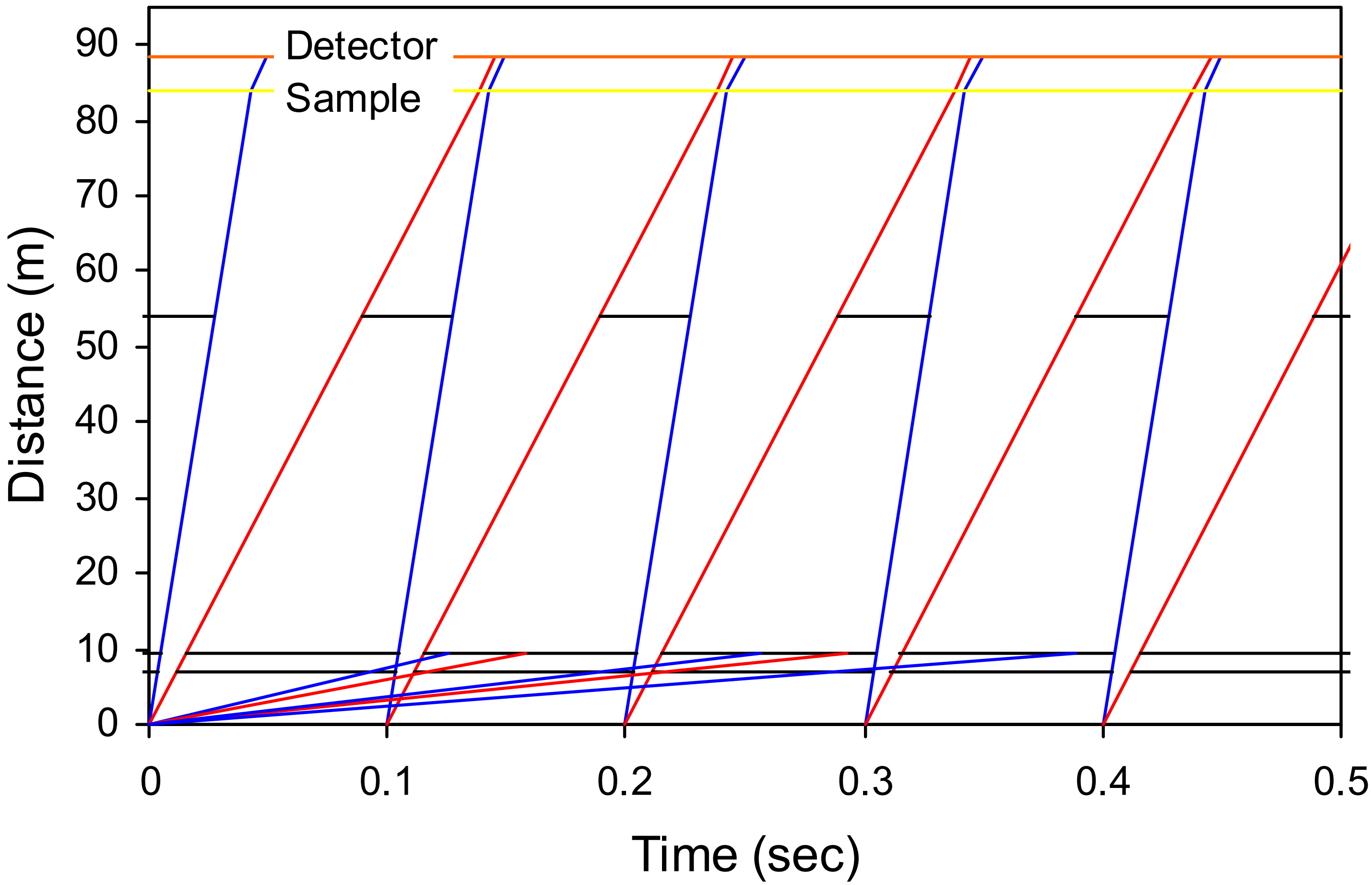
Chopper Timing Diagram



Resolution Function - Energy resolution

$$\omega = E_i - E_f$$

$$E_i = \frac{5.227 \text{ x } 10^{-6} L_1^2}{\left(t - t_f\right)^2}$$

$$\delta E_i = 2E_i \left[\frac{\left(\delta L_1\right)^2}{L_1^2} + \frac{\left(\delta t\right)^2}{\left(t - t_f\right)^2} + \frac{\left(\delta t_f\right)^2}{\left(t - t_f\right)^2} \right]^{1/2}$$

$$E_f = \frac{81.8}{\lambda_f^2} = \frac{81.8}{4d^2 \sin^2\left(\theta_B\right)}$$

$$\delta E_f = 2E_f \left[\frac{\left(\delta d\right)^2}{d^2} + \cot^2\left(\theta_B\right) \times \left(\delta\theta_B\right)^2 \right]^{1/2}$$

Uncertainty in emission time from moderator

$$\delta\omega = \left[\left(\delta E_i\right)^2 + \left(\delta E_f\right)^2 \right]^{1/2}$$

$$t_f = \frac{L_2 2d \sin\left(\theta_B\right)}{3956}$$

$$\delta t_f = t_f \left[\frac{\left(\delta L_2\right)^2}{L_2^2} + \frac{\left(\delta d\right)^2}{d^2} + \cot^2\left(\theta_B\right) \times \left(\delta\theta_B\right)^2 \right]^{1/2}$$

Backscattering on Short-Pulse and Long-Pulse Source

- BaSiS at the SNS has a moderator pulse width at λ = 6.27 Å (elastic wave length) of about 60 μsec (fwhm), L_1 = 84 m ($L_2 \approx$ 4.25 m). Consider the moderator timing contribution (essentially how well we know the incident neutron wavelength)

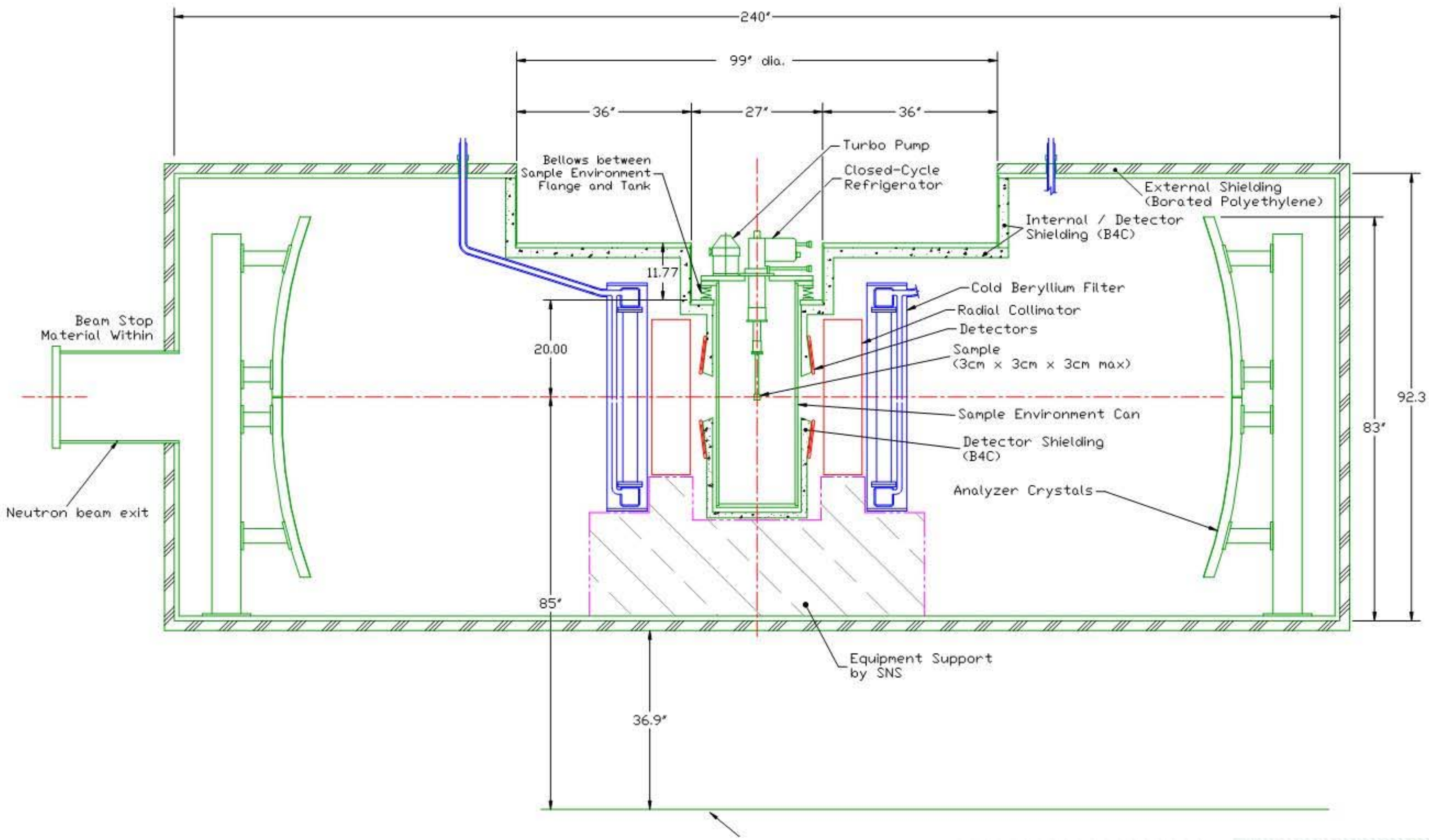
$$\frac{(\delta t)}{(t-t_f)} = \frac{60\times10^{-6}\ \mathrm{s}}{133{,}000\times10^{-6}\ \mathrm{s}} = 4.5\times10^{-4}$$

- BaSiS has a wavelength bandwidth of

$$\Delta\lambda = \frac{3956(1/\mathit{frequency})}{L_1} = 0.785\ \text{Å}$$

- At the 14 Hz frequency of the ESS, this $\Delta\lambda$ implies that the instrument would be 360 m long. At 300 m, $\Delta\lambda$ = 0.94 Å, the fast chopper pulse width could be 214 x 10^{-6} s and placed 12 m from the moderator to give $\Delta\lambda$ = 0.94 Å from a 2.86 x 10^{-3} s source pulse.

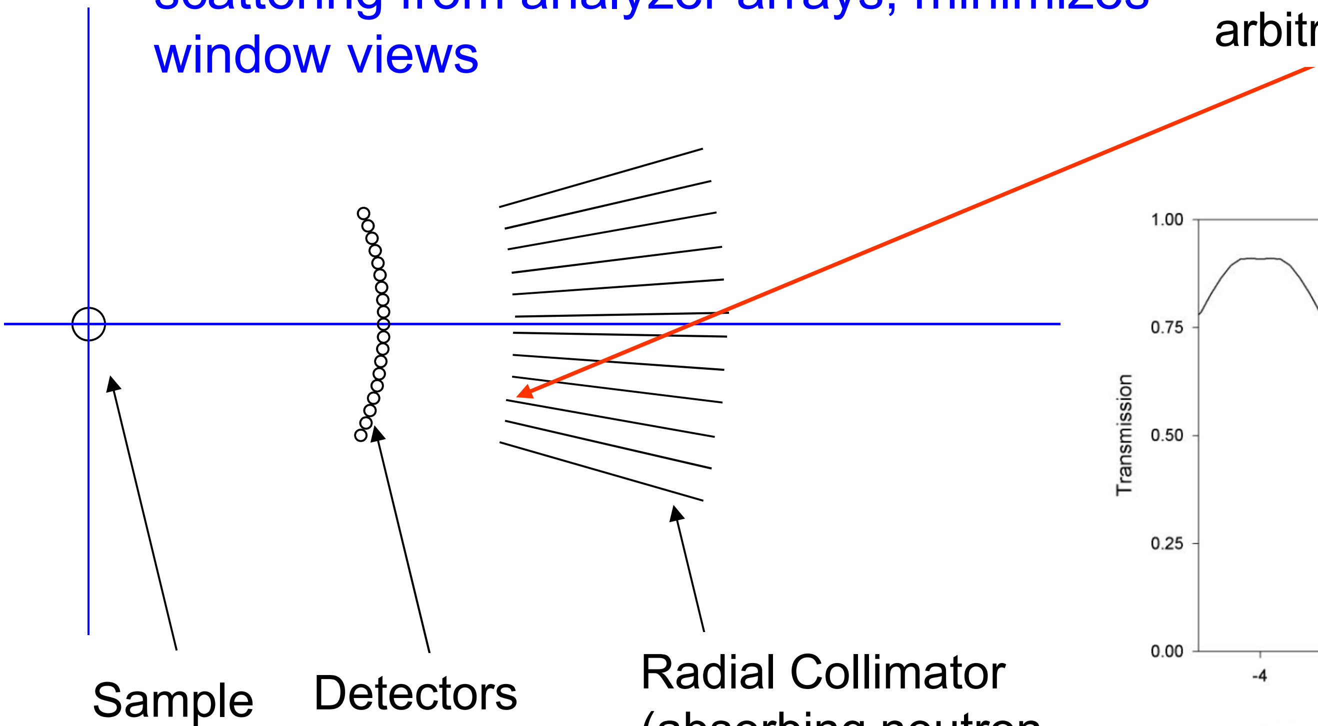
Background Reduction – improving Signal-to-Noise

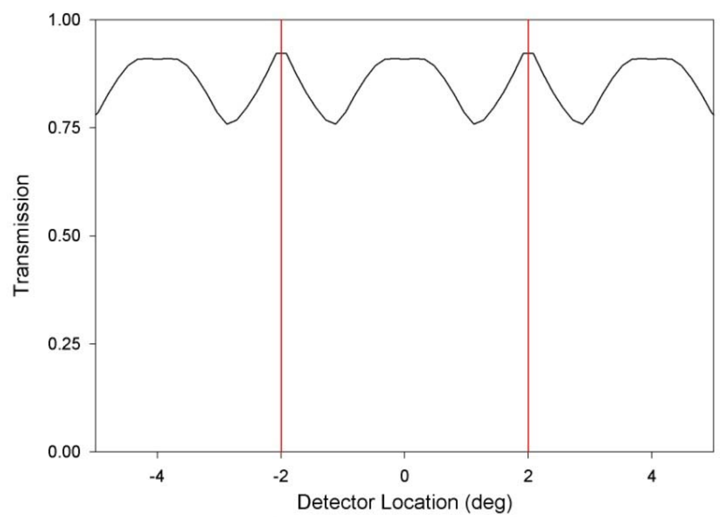


Radial Collimator

Factor of 20 reduction in non-Bragg scattering from analyzer arrays, minimizes window views

Non-Bragg scattered neutron, returning as an arbitrary ray from analyzer





Net transmission, final design 4 deg blade separation 20 cm blades

Summary

- Define the science capability – translate into technical requirements – translate into engineering design
- You heard about
  - The interplay between: distances, time, source frequency, band width, choppers, timing diagrams
  - Short and long-pulse realization of instruments
  - Signal-to-noise optimization
- Some things we did not discuss
  - Shielding
    - Beam line shielding - massive and expensive – especially close to spallation source
    - Detectors – high cross-section neutron absorbers – B, Cd, Gd, Li, ^{3}He – physical size/pixelation, timing resolution
  - Guide optimization – how much phase space do you need and how efficiently can you transport it the required distance (interplay between neutron transport and wavelength resolution).
    - Phase Space Diagrams
    - Monte Carlo
  - Focusing elements – mirrors, lenses, “trumpets”, crystals(Bragg reflection)
    - Beam compression to enable faster chopping

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Where can I learn more?

- Repetition Rate/Wavelength Frame Multiplication
  - M. Russina, et al., Nucl. Instrum. Meth. A **654**, 383-389 (2011)
- Time-focusing
  - J. M. Carpenter, Nucl. Instrum. Meth. A **483**, 774-783 (2002)
  - J. M. Carpenter, et al., Nucl. Instrum. Meth. A **483**, 784-806 (2002)
- More about BaSiS – the near backscattering spectrometer at the SNS
  - K. W. Herwig and W. S. Keener, Appl. Phys. A **74**, S1592-S1594 (2002).
  - E. Mamontov and K. W. Herwig, Rev. Sci. Instrum. **82**, 85109 (2011).
- SoNS – 2016 Erice School on Designing and Building a Neutron Instrument - http://www.sonsfpricci.org/school-sons-2016

SNS Second Target Station

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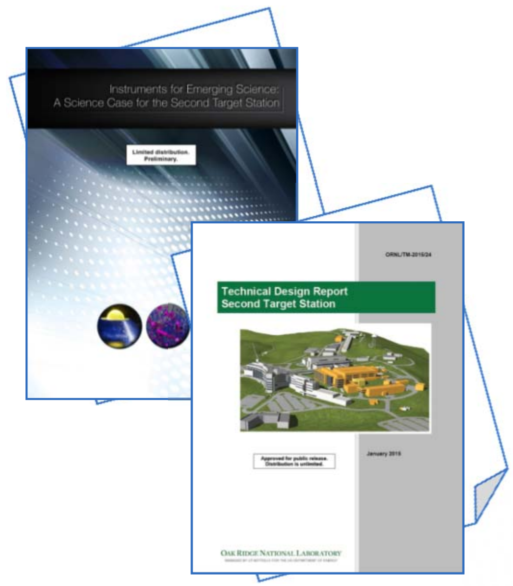
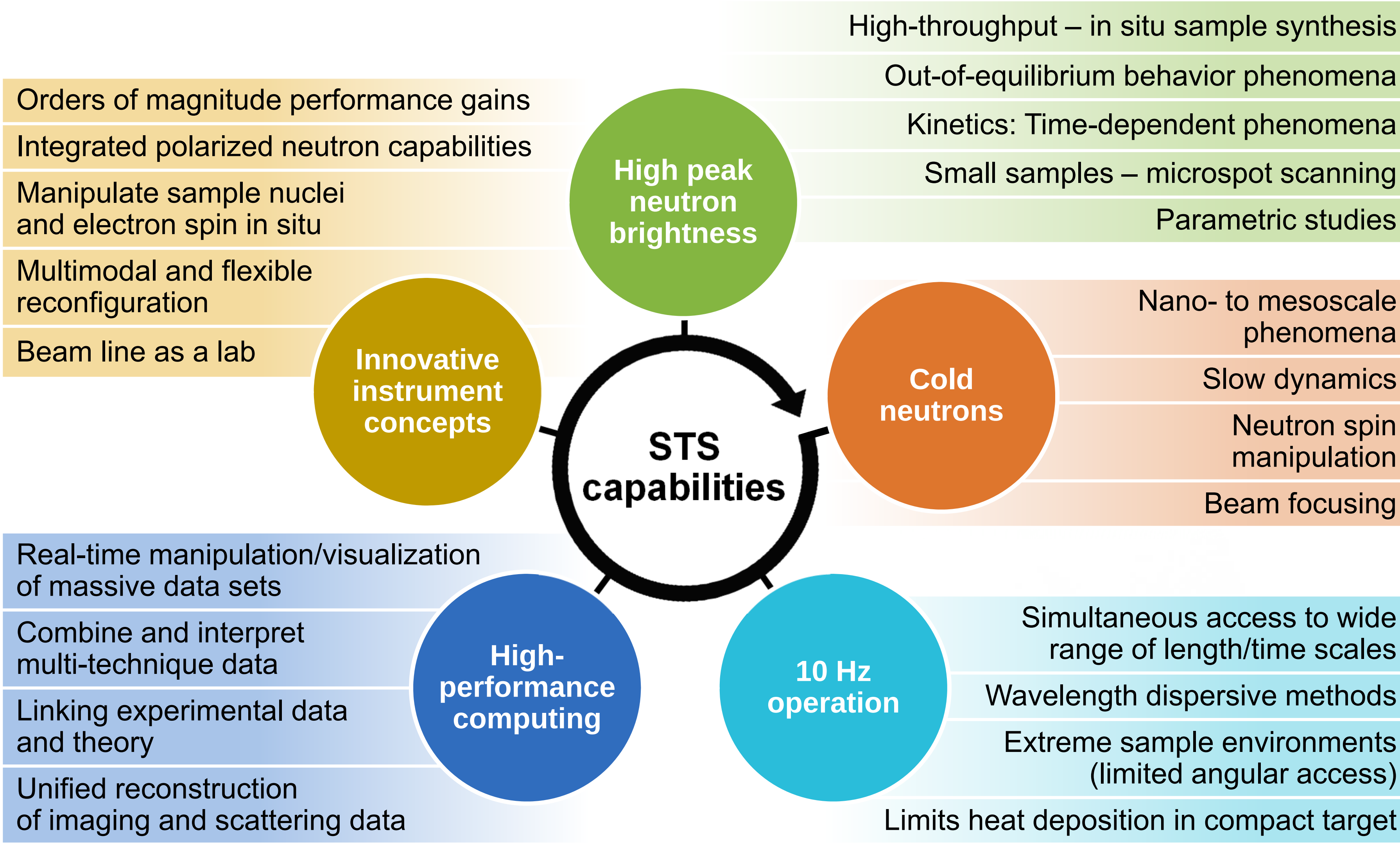
Identifying emerging scientific challenges and technical solutions to address user needs

December 2013–March 2015	October 2014	October 2015
Workshops with scientific community representatives to identify Grand Challenges for Neutrons	ORNL staff and external experts construct draft Technical Design Report (TDR) and science case	STS user meeting organized by the SNS-HFIR User Group develops instrument needs and selects 12 instruments to be considered for further design

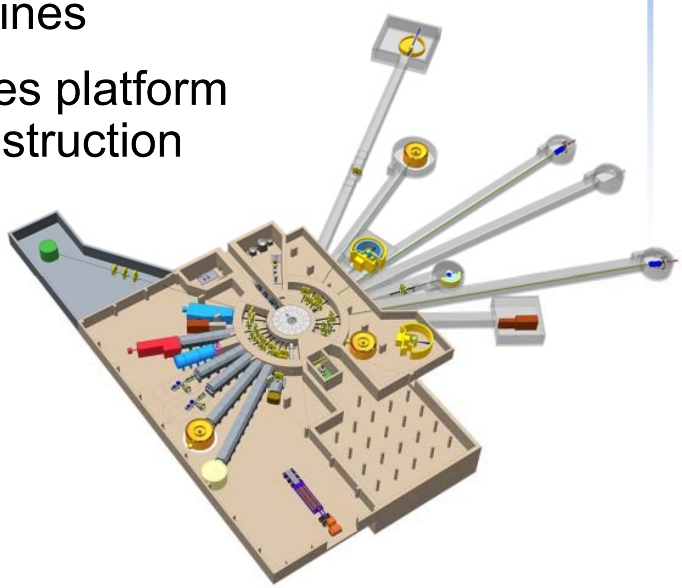


Innovative STS design enables new science to meet BES needs



STS / PPU: Single Mission, Separate Projects

SNS-PPU	SNS-STS
• Increases power capabilities of existing 60 Hz accelerator structure from 1.4 MW to 2.8 MW • Increases power delivered to first target station (FTS) to 2 MW • Increases neutron flux on available beam lines • Provides platform for construction of STS	• Initial suite of 8 beam lines, with capacity to accommodate 22 beam lines • 467 kW diverted to STS by additional accelerator systems • 10 Hz repetition rate, enabling broad dynamic range • World's highest brightness short-pulse source optimized for cold neutrons • 380,000 ft^2 of new infrastructure



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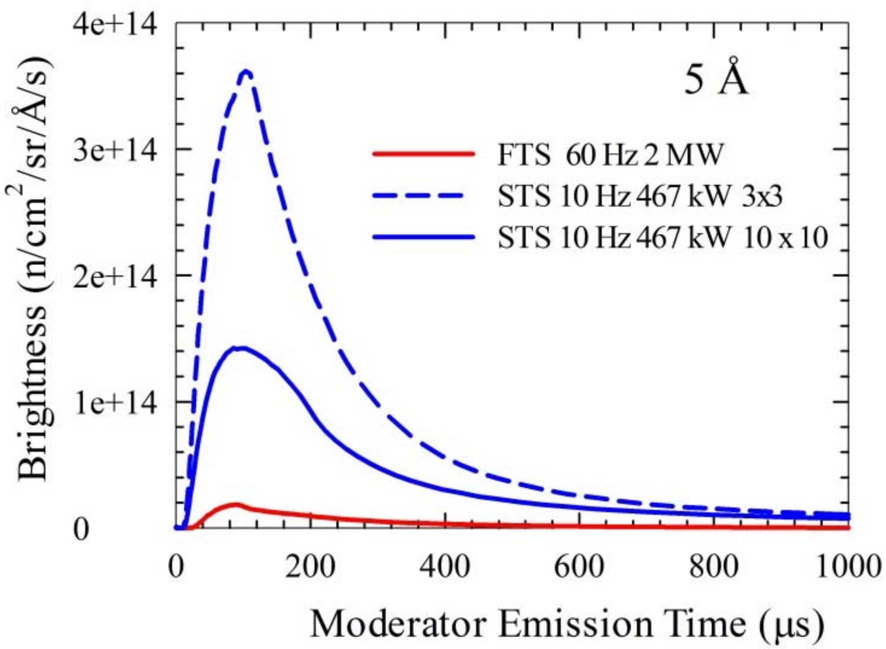
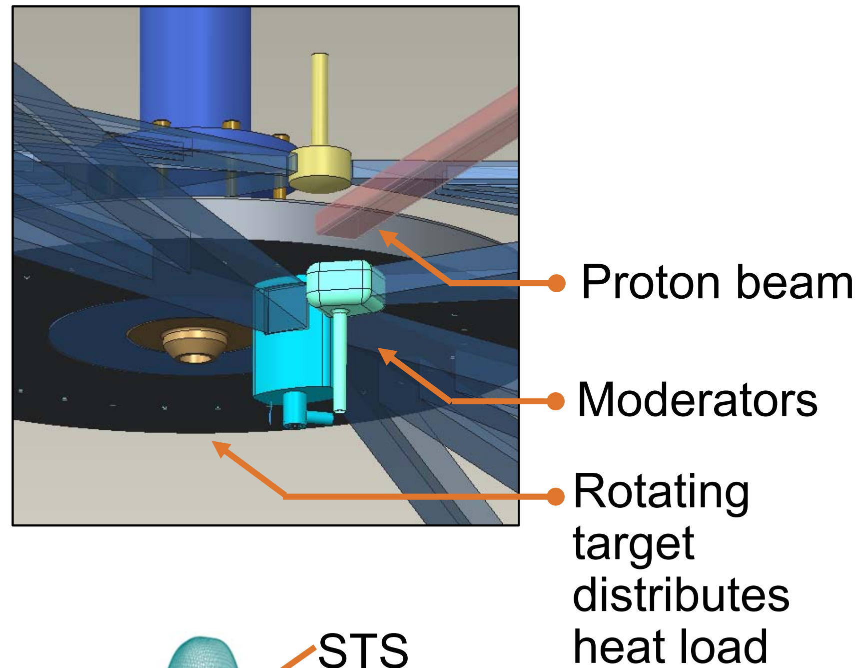
STS is optimized for highest neutron peak brightness at long wavelengths

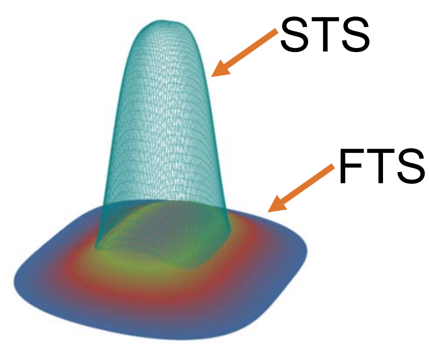


STS: 20× FTS

- Optimal moderator placement: 2×
- Compact neutron production zone: 4×
- Moderator geometry: 2.5×

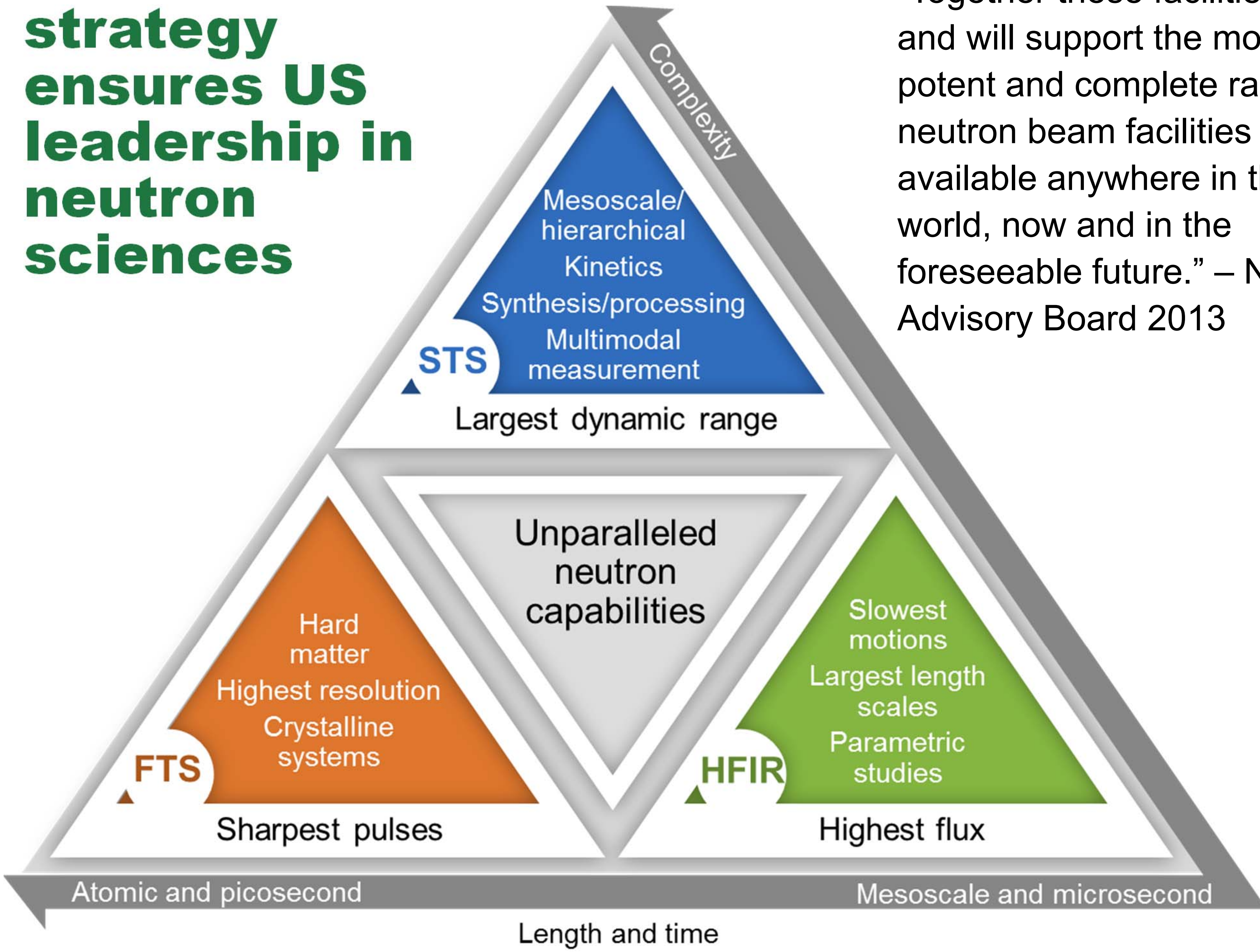
2016 – adopted rotating target
(option for higher source frequency/power)





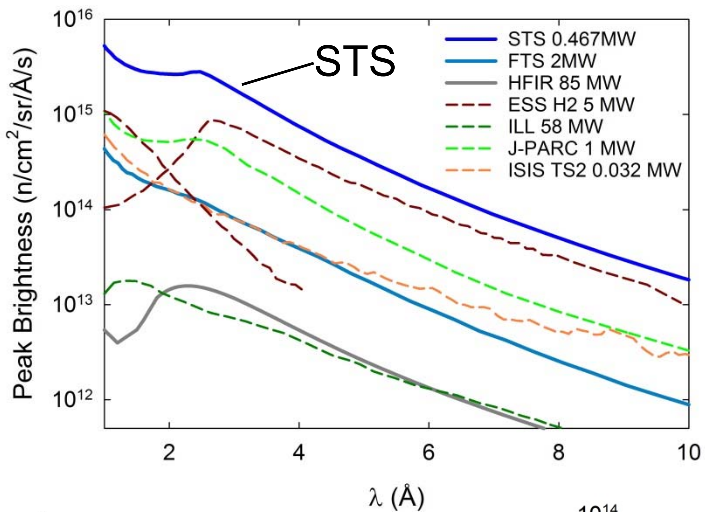
Proton beam footprint

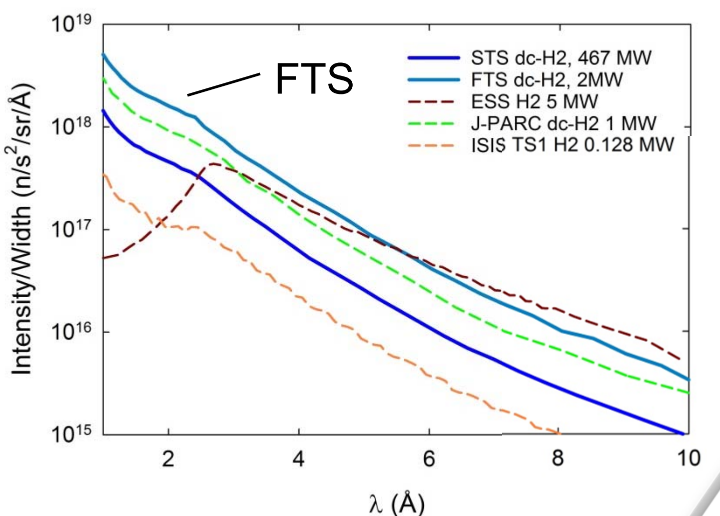
Three source **strategy ensures US leadership in neutron sciences**

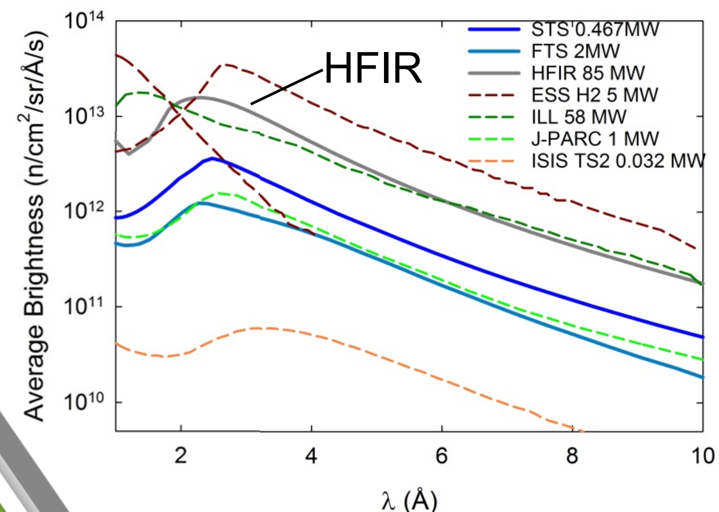


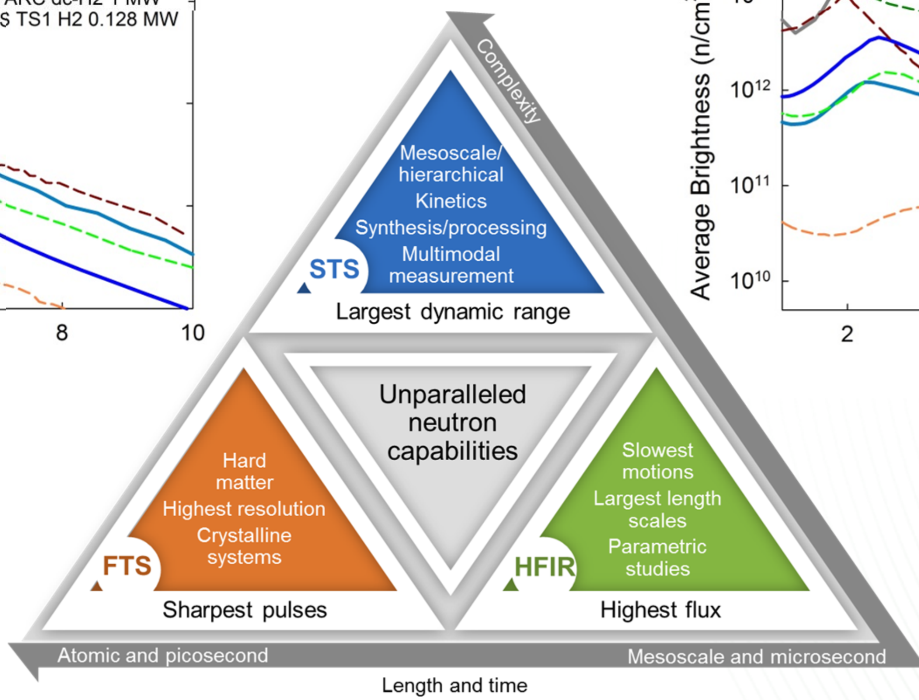
"Together these facilities can and will support the most potent and complete range of neutron beam facilities available anywhere in the world, now and in the foreseeable future." – NScD Advisory Board 2013

Three source strategy ensures US leadership in neutron sciences



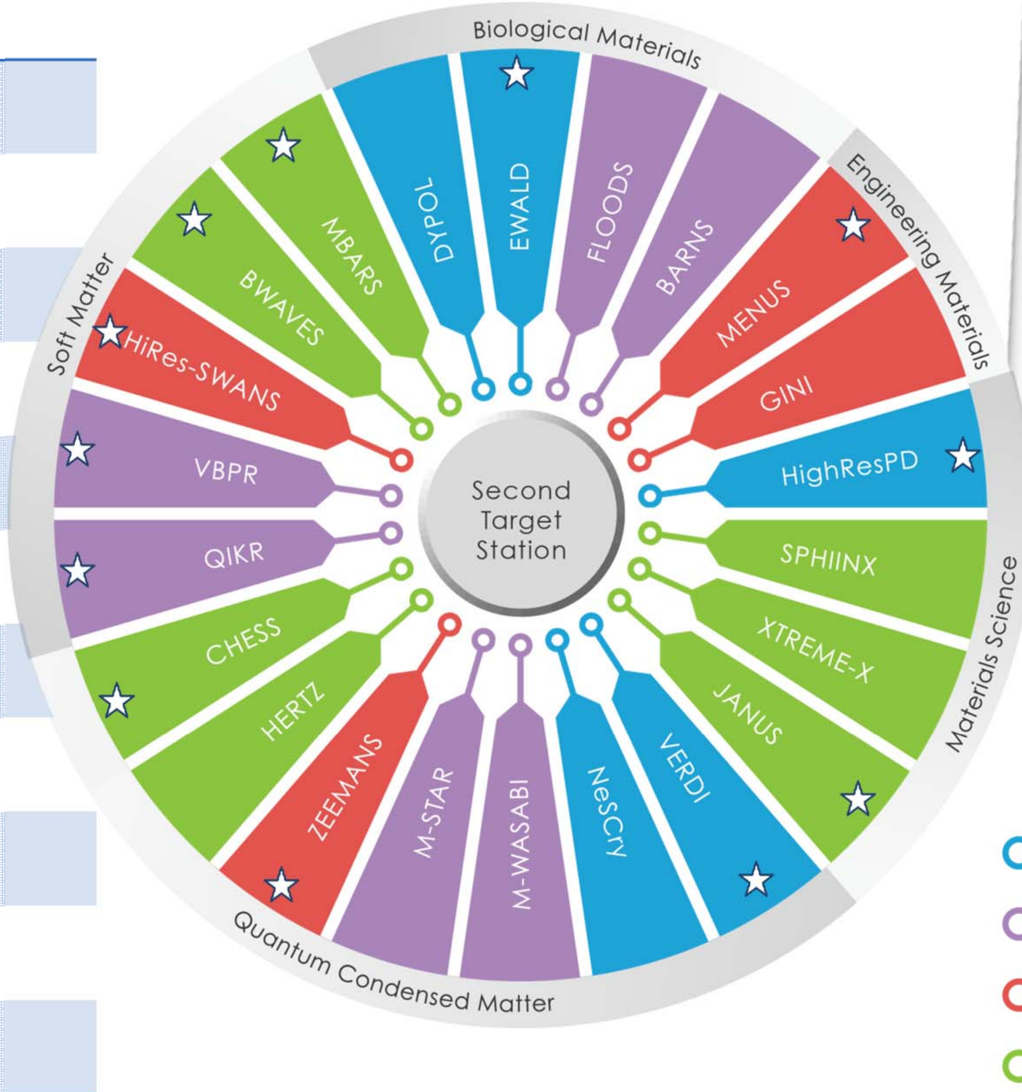


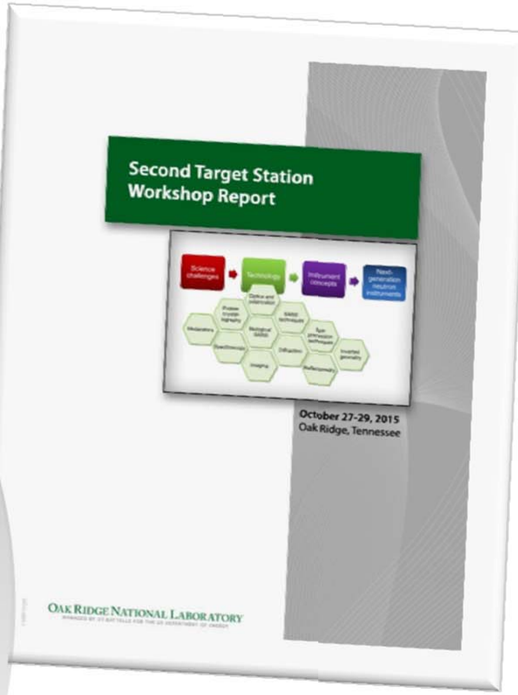




User community identified 12 high-priority instruments – October 2015

MBARS
BWAVES
JANUS
CHESS
ZEEMANS
MENUS
EWALD
VERDI
HighResPD
HiRes-SWANS
QIKR
VBPR





STS Instruments FY16-FY17

- Concept development – initial neutron optics designs – Monte Carlo models – instrument figure-of-merits
  - QIKR (kinetics reflectometer) – John Ankner and Tim Charlton
  - HiRes-PD (100 m powder diffractometer)– Uli Wildgruber
  - EWALD (Macromolecular single-crystal with dynamic nuclear polarization) – Leighton Coates
  - CHESS (small sample cold neutron chopper spectrometer)– Georg Ehlers
  - ZEEMANS (high magnetic field multi-modal) – Barry Winn (magnet technology)
  - FY17 – initiate 5 more from top 12 list
- Moderator Optimization – explore production of 10-30 Å neutrons
- Instrument integration with target monolith and conventional facilities
- Detector needs evaluation (white paper)
- Analyze instrument performance as a function of source frequency and pulse shape (duration) – following the recommendation from the BESAC facility prioritization sub-committee
- **Regional science-themed workshops – 3 to 4 per year**
  - **Engage community in identifying a set of exciting "first experiments" for STS**
  - Simulate early science experiments at STS

Where do all the neutrons go?

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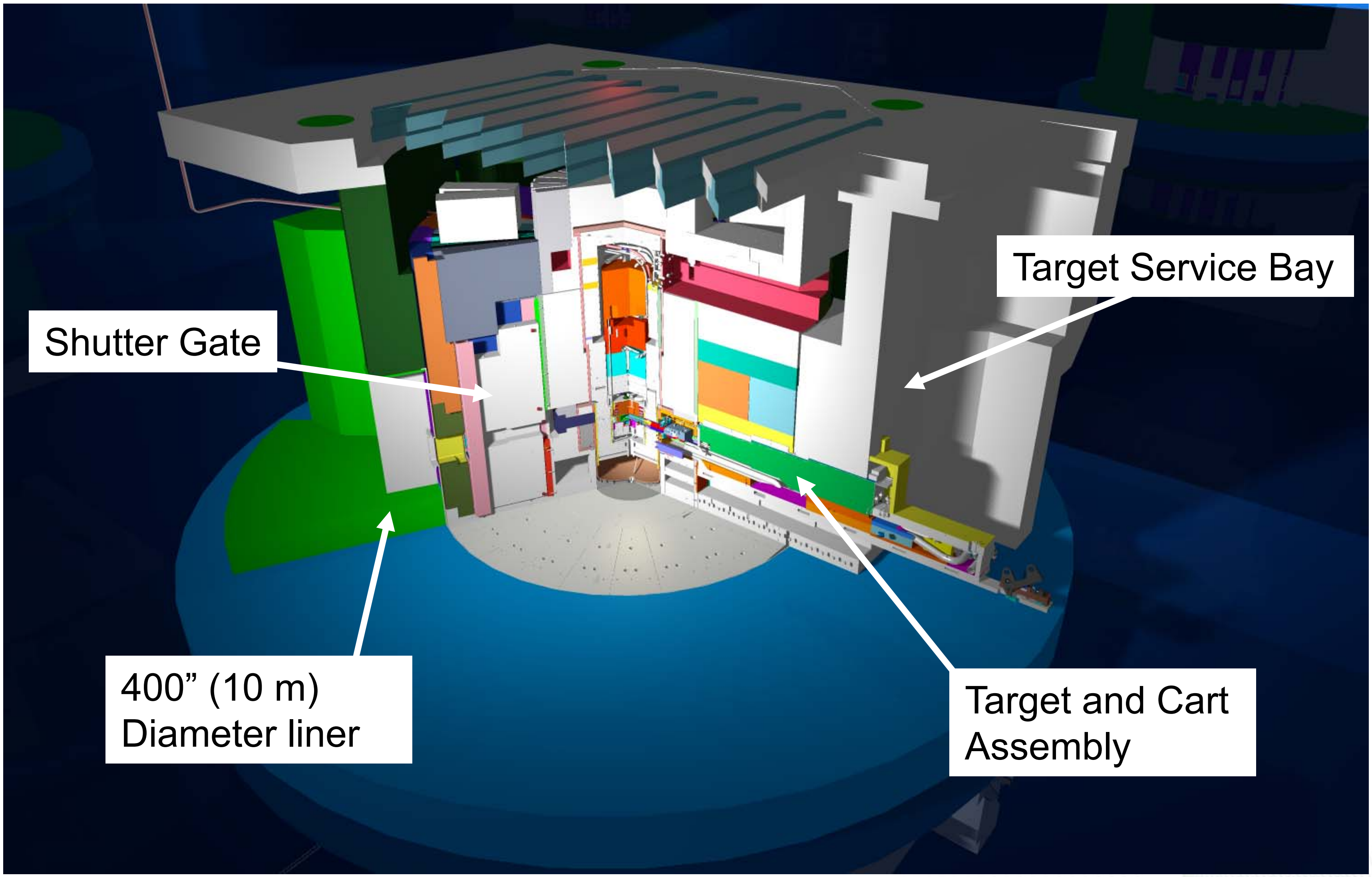
SNS Target Monolith



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Where do all the neutrons go?

Systems	Production (n/p)	Capture (n/p)
Target Module	21.7 (85%)	5.1 (20%)
Moderator System	0.1	2
Inner Reflector Plug	2.4 (9%)	8.8 (34%)
Outer Reflector Plug	1	5.9 (23%)
Proton Beam Window	0.4	0.4
Total	***25.6***	22.2

2.1 n/p are deposited into the shielding
1.3 n/p (5%) exit the outer reflector (1m radius) towards the instruments

How many neutrons does SNS make in a year?

- 26 neutrons/ 1 GeV proton
- SNS at 1 MWatt
  - 1 GeV protons @ 1 mA (time averaged) (approx. $1.04 \cdot 10^{14}$ protons/pulse, 60 Hz)
- Neutrons/sec = 26 x $6.24 \cdot 10^{15}$ = $1.6 \cdot 10^{17}$ n/sec
- Neutrons/year (5000 hours) = $2.9 \cdot 10^{24}$ = 4.8 moles/year

How many neutrons do we count on BaSiS – the near backscattering spectrometer?

- Guide transmits about $2 \cdot 10^7$ n/sec to sample
- 10% scattering sample into $4\pi = 2 \cdot 10^6$ n/sec
- Analyzer is 1.2 sr, 10% scattered neutrons reach analyzer = $2 \cdot 10^5$ n/sec
- Analyzer accepts about 0.004, reflecting back to detectors = 800 n/sec
- There is some loss in radial collimator 80% transmission so count about 600 n/sec
- SNS produces about $1.6 \cdot 10^{17}$ n/sec
- BaSiS counts $4 \cdot 10^{-15}$ of the neutrons produced at SNS
- Some instruments count at much higher rates (~10^6 counts/sec) and there are 24 instrument stations so <1.5 10^{-10} of the neutrons are counted across all instruments

Questions?

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