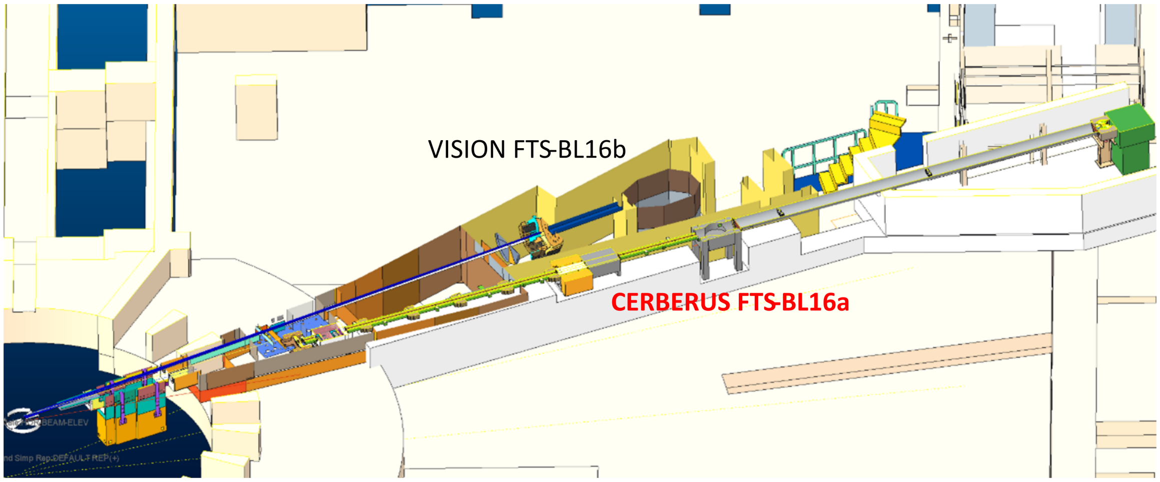
ORNL/TM-2023/2823

CERBERUS: A Multi-Purpose Spectrometer and Alignment Station at SNS



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January 2023

OAK RIDGE National Laboratory

ORNL IS MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY

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Neutron Technologies Division, Neutron Sciences Directorate

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ABBREVIATIONS

Å	Angstrom
AC	Alternating Current
ATR	Advanced Test Reactor
BL	Beamline
BW	Bandwidth
CCD	Charge Coupled Device
CCR	Closed Cycle Refrigerator
CNMS	Center for Nano-phase Material Sciences
DSP	Digital Signal Processor
ENDF	Evaluated Nuclear Data File
eV	electron-Volt
FEM	Front End Module
FTS	First Target Station
FWHM	Full-Width at Half-Maximum
GUP	General User Program
HD	High Density
HFIR	High Flux Isotope Reactor
HVAC	Heating Ventilation and Cooling
JEFF	Joint Evaluated Fission and Fusion
JENDL	Japanese Evaluated Nuclear Data Library
LPSD	Linear Position Sensitive Detector
MC	Motor Control
MCNP	Monte Carlo N-Particle
ND	Nuclear Data
NIR	Near-Infrared
NScD	Neutron Sciences Directorate
ODB	Optical Distribution Board
ODH	Oxygen Deficiency Hazard
ORELA	Oak Ridge Electron Linear Accelerator
ORNL	Oak Ridge National Laboratory
PG	Pyrolytic Graphite
PPS	Personnel Protection System
PPU	Proton Power Upgrade
SAMMY	Not Defined, Name of a Computer Code
SCALE	Standard Computer Analysis for Licensing Evaluation
SCW	Sensible Chilled Water
SD	Standard Density
SNS	Spallation Neutron Source
TOF	Time of Flight

ABSTRACT

In order to maximally utilize the existing beam ports at the Spallation Neutron Source, development and installation of a new neutron instrument is proposed for beam port 16a within building 8700 at Oak Ridge National Laboratory. Said instrument will provide nominally equal neutron beam access for three main science purposes; (1) as an alignment station for proposed single-crystal spectrometer samples to be run across the facility, (2) as a Near-Infrared (>100meV) filter analyzer spectrometer, nearly identical to that which was previously housed at the Lujan Center in Los Alamos, and (3) as a high-throughput nuclear cross-section measurement station. These three experimental applications would require no substantial technical developments, are complimentary in their technical requirements, and provide a worth-while capability that is infinitely beyond the current use of the 16a beam port at the First Target Station within the SNS complex. All three methods would enhance the facility's science contributions, while accommodating two niche experiment methods that may not be strong enough to stand on their own.

1. INTRODUCTION

The General User Program housed within the Neutron Sciences Directorate at Oak Ridge National Laboratory utilizes two intense neutron sources to provide scientists from all over the world an instrument suite to characterize quantum, chemical, engineering, and biological materials with unprecedented speed and resolution. In addition, those same instruments have been used to support fundamental neutron physics experiments and the development of novel neutron optics and detectors. In order to maintain a world-class neutron scattering capability, continual improvement in instrumentation technologies and experimental focus is absolutely essential. CERBERUS can enable that continual improvement by expanding science capabilites and support at the First Target Station of the Spallation Neutron Source.

2. SCIENCE CASES

CERBERUS is designed to support the crystal alignment needs of the user program while at the same time expanding its science portfolio to include neutron cross-section measurements and mid/short/near-infrared spectroscopy experiments. The current limitations of the facility in supporting these three experimental capabilities and the potential gains that can be added to ORNL's user facilities by CERBERUS will be described in this section.

2.1 ALIGNMENT STATION

The SNS performs materials experiments that need off-line alignment at an average rate of nearly 30 proposals per year. Currently, the burden of aligning samples is supported by a dedicated alignment station at HFIR. This dedicated station is not always available when needed, as SNS and HFIR do not run on the same schedule. Furthermore, anticipated upgrades to be installed at HFIR during the latter half of the 2020's will create a gap in support exceeding a year or more. During this time, science involving Bulk Magnetism, Quantum Materials, and Energy Materials will suffer since crystal alignment will need to be performed in situ, causing beam time losses during each experiment. Clearly, the alignment station provides a substantial operational benefit to the user program and any internal science initiatives that rely on sample alignment and quality confirmation.

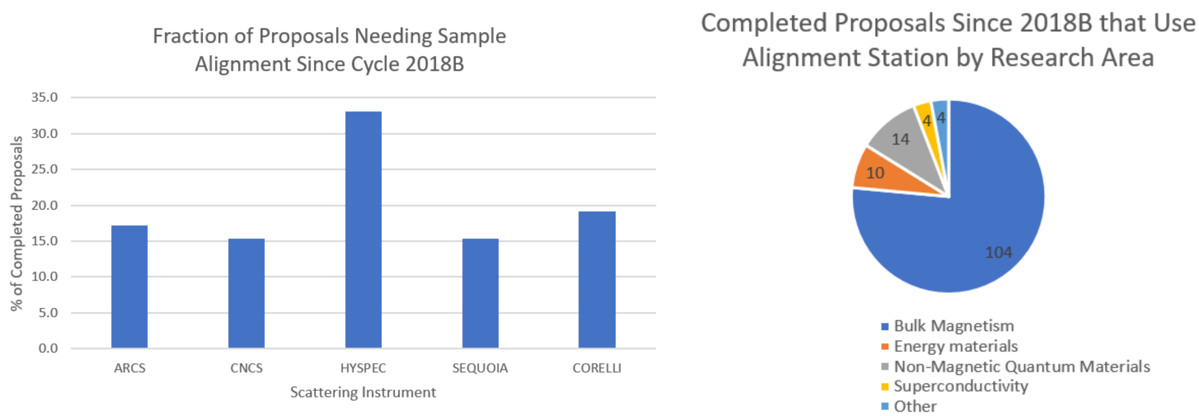

Figure 1. Charts created from data mined from the Integrated Proposal Tracking System (ipts.ornl.gov). On the left, percentage of total proposals on each TOF instrument at the SNS that used the alignment station since run cycle 2018B. To the right, a pie chart describing the range of science impacted on those same instruments by the use of the HFIR alignment station since run cycle 2018B.

2.2 BeFAST SPECTROMETER

VISION, the vibrational spectroscopy instrument at FTS-SNS utilizes pyrolytic graphite (PG) crystals on its scattering arms in conjunction with an incident white-beam to resolve energy transfer in the range of 10 to 1000meV. The neutron energy bandwidth reflected by these crystals is on the order of 0.1 meV, and as a result the signal at higher energy transfers is depleted immensely. Thus, the need for a different but complimentary spectrometer whose energy resolution may be poorer, but whose performance is substantially improved in the near-infrared energy transfer regime. BeFAST, a spectrometer that uses low-pass energy filtering rather than narrow energy selection by diffraction scattering is a solution, providing an increase in the signal at those higher energy transfers by 20 to 50 times. This is a capability that is currently offered at other world-class neutron scattering facilities such as ANSTO, NCNR and LANSCE.

Besides complementing VISION, BeFAST will also allow for new avenues of scientific research at SNS by enabling neutron near-infrared (NIR) spectroscopy, as the current TOF spectroscopy instruments do not have the range required to meet these needs, as seen in Figure 2. The frequency range above 4,000 cm^{-1} is particularly rich in overtones and combination bands. These transitions occur in large part because of bond anharmonicity. Bonds involving hydrogen and some other heavier elements such as oxygen, carbon, nitrogen, or sulfur (i.e., O-H, C-H, N-H, and S-H bonds) tend to present high anharmonicity and high bond energy with fundamental vibrational transitions in the 3,000–4,000 cm^{-1} range. It follows that overtones and combinations in the fundamental vibrations of such bonds occur in the spectral range associated with NIR. This energy range is of interest to members of the catalysis community, since many catalytic reactions involve making and breaking C-H bonds, which have stretching frequencies in the range of 2,800–3,300 cm^{-1}, and many oxide surfaces (and alcohols) have O–H stretches in the 3800–3500 cm^{-1} region. As the science case for BeFAST is developed, it will be important to engage the catalysis community to ensure this instrument addresses this critical science theme.

The extraction of reliable anharmonic parameters is important for computational chemistry, for example in the development of force fields for molecular mechanics or to refine approaches to the reliable computation of vibrational spectra and properties depending on the vibrational density of states. Currently, insufficient experimental data are available, and optical selection rules limit the usefulness of Raman or Fourier

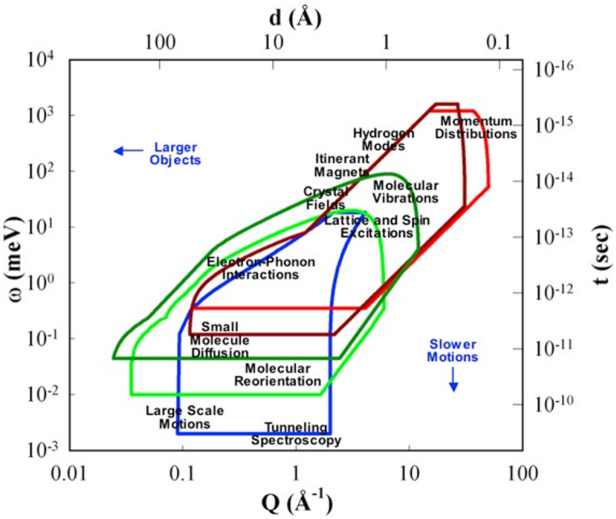

Figure 2. A chart describing the current spectroscopic capability at SNS. Specific instrument ranges are defined as follows: ARCS in red, SEQUOIA in dark red, HYSPEC in dark green, CNCS in green, and BASIS in blue. Absent is VISION which would cover the molecular vibration range. The proposed BeFAST configuration for CERBERUS would cover the hydrogen mode range. Plot courtesy of Georg Ehlers.

transform infrared spectroscopy, particularly with small, highly symmetric molecules. Neutron NIR spectroscopy is not subject to this constraint. Accurate anharmonicity information will also allow researchers to calculate accurate potential energy surfaces, a conceptual tool used in the analysis of reaction dynamics. Such calculations for realistic reactions and models are now within the reach of supercomputers, and experimental NIR neutron vibrational data will be needed to develop this important field of reaction dynamics. Co-located optical spectroscopy and theory/modeling capabilities at CNMS will add additional value to the instrument's user community.

An important scientific area that would benefit greatly from the availability of neutron NIR vibrational data is water and other hydrogen-bonded systems. Water is present in materials in many forms. Its structure and dynamics, whether in the pure state or in various other forms, continue to be the object of numerous studies. Because of strong hydrogen bonding, water is strongly anharmonic. Access to a filter spectrometer with usable intensity in the NIR range will provide information on water anharmonicity to researchers in the fields of biology, chemistry, geology, environmental science, and materials science. More generally, anharmonic, hydrogen-bonded molecular entities are associated with important physical behaviors such as glass formation or energy transfer and localization in proteins.

2.3 NEUTRON INDUCED CROSS-SECTION STATION

Neutron/nucleus cross-section measurements are of great value to both science experiment and instrument technology applications at NScD's sources. Understanding the energy-dependent interactions a neutron has with materials is integral to neutron radiography and traditional scattering experiments, as well as an important input to complex safety simulations used to determine radiological and background performance of shielding in instrument designs. Modeling and simulations of any nuclear application using codes such as SCALE or MCNP rely on the quality of the existing evaluated nuclear data libraries such as Evaluated

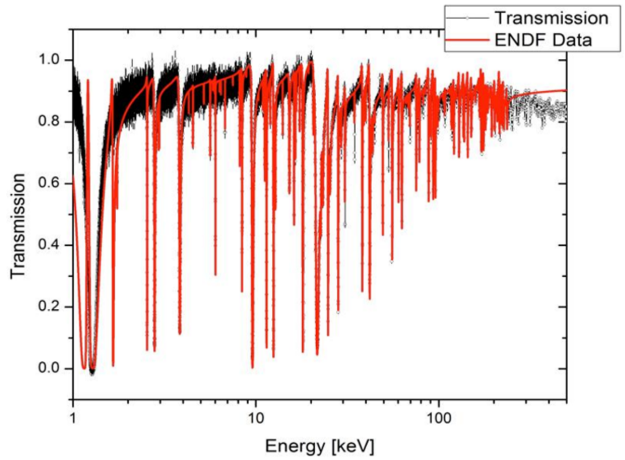

Figure 3. Natural Cerium transmission data, compared to the Cerium ENDF Library. Data such as this is limited in availability for many elements in energy regimes accessible at BL16A.

Nuclear Data File (ENDF)/B, the Joint Evaluated Fission and Fusion (JEFF) nuclear data library, or the Japanese Evaluated Nuclear Data Library (JENDL). In some cases, the cross-section evaluations of those libraries were found to be deficient in accurately describing criticality benchmarks, to name just one example. Furthermore, those libraries have gaps in neutron induced cross section data of radioactive isotopes (actinides and fission products) and rely in many cases on theoretical calculations or estimations. Modern simulation codes are capable of handling covariance data but the lack of these for radioactive isotopes can create large uncertainties in those calculations.

Furthermore, nuclear data (ND) experimental capabilities will expand ORNL's scientific portfolio by providing the ability to perform cross-section measurements of radioactive nuclei and to provide additional cross-section information that is important to understanding heavy-element nucleosynthesis processes within unique stellar phenomena. Advanced reactor development projects also need cross section information on long-lived fission products which can potentially be a neutron poison. This new cross section information on radioactive isotopes will support the DOE Isotope production program, radiological shielding calculations, and burn up credit for reactor simulations. Homeland security focused projects can be supported by providing basic experimental capabilities towards the development of non-destructive assay techniques, nuclear non-proliferation, and novel sensing of special nuclear materials.

Performing ND experiments at SNS aims to develop further the synergies at ORNL by enhancing experiments using the HFIR irradiation system and hot cells for short to long-lived radioactive sample production. This, in combination with the high flux of SNS obtained from the thermal water moderator, will enable neutron induced cross section experiments on small radioactive samples in μg to mg quantities. The high neutron flux will enable examination of small samples which is beneficial for radiological protection concerns and mitigates the difficulties encountered in harvesting enough material to perform a good measurement. The SNS facility at ORNL is uniquely suited to provide these measurements as the neutron flux is approximately 10-20 times greater than comparable sources at other US facilities assuming current accelerator conditions. After the Proton Power Upgrade (PPU) project is complete, the flux is expected to be an additional 40% greater.

3. ANTICIPATED USER COMMUNITY AND FEDERAL SUPPORT

An instrument is only as productive as the user community that it intends to cultivate and support over its lifetime. CERBERUS is designed to cater to a very wide community of users, and at the same time provide new avenues of science experiment support at ORNL.

3.1 ALIGNMENT STATION

Alignment stations are an integral component to any scattering facility. The one that is currently housed at HFIR is used for nearly all single-crystalline based spectroscopy measurements. HFIR does not run every day of the year, and our organization anticipates a substantial interruption in neutron reactor production due to planned upgrades. The loss of that alignment station would create a significant burden on already precious spectrometer beam time. CERBERUS can fill this gap in the short-term and provide an additional means by which to align samples in the long term.

3.2 FILTER DIFFERENCE SPECTROMETER

As noted in the science case, BeFAST would complement VISION but also open avenues into materials focused on catalysis and water-bonded systems. This is a user community that is not supported in our current instrument suite, and therein lies an opportunity to expand the user program with unique collaboration opportunities for the directorate.

3.3 NEUTRON INDUCED CROSS-SECTION EXPERIMENTS FOR NUCLEAR DATA

Providing a high-accuracy cross-section measurement station would open up new scientific avenues for the user facilities at ORNL. With the high flux of the SNS, experiments that have been up to now very difficult or impossible to perform are within reach. There are several DOE offices who have a vital interest in Nuclear Data (ND) for radioactive isotopes. The need is of a wide variety ranging from isotope production, homeland security, nonproliferation to nuclear energy and basic science. Of particular note is the need to support ND for isotope production in nuclear reactors as published in the DE-FOA-0002440. These needs are conveyed in Table 1.

Many of these reaction and data needs can be satisfied via total cross section and fission cross section experiments. The low hanging fruit on this list is the search for the postulated resonance at 1 eV for ^{252}Cf, which could easily be confirmed by a high-intensity transmission experiment at the proposed beamline. The Office of Nuclear Energy has emphasized the need for long-lived fission product cross-sections for advanced reactors in the epithermal neutron energy range, in particular neutron capture on ^{85}Kr, ^{89,90}Sr, ^{91}Y, ^{95}Nb, ^{93,95}Zr, ^{99}Tc, ^{107}Pd, ^{115}Cd, ^{129,131}I, ^{125}Sb, ^{134,135,136,137}Cs, ^{133}Xe, ^{140}Ba, ^{141}Ce, ^{143}Pr, ^{147}Nd, ^{147}Pm, ^{155,155}Eu, and ^{151}Sm. In some cases, capture cross-sections can also be inferred from resonance parameters obtained via transmission experiments and Hauser-Feshbach statistical model calculations.

In addition to providing information about cross sections of novel nuclei and supporting nuclear data acquisition campaigns, this instrument mode can provide information that is critical to understanding materials to be imaged at HFIR and SNS. Convenient access to such a resource makes experiment preparation more straight forward for users and local instrument staff to ensure the best use of beam time on the other instruments. One sees CERBERUS providing additional capability for any user interested in radiographic imaging with epithermal, thermal or cold neutrons.

Table 1. Low energy neutron reactions: Isotope production via reactors. Energy-resolved cross sections as well as effective cross sections for both thermal and epithermal neutrons are needed for production at U.S. based reactors (e.g. HFIR and ATR).

Nuclear reaction	Nuclear reaction	Nuclear reaction
Data for production of ^{229}Th and other isotopes ^{227}Ra(n,y)^{228}Ra - confirmation measurement needed ^{228}Ra(n,y)^{229}Ra ^{228}Ac(n,y)^{229}Ac ^{227}Th(n,y)^{228}Th - confirmation measurement needed ^{228}Th(n,y)^{229}Th - confirmation measurement needed ^{229}Th(n, y)^{230}Th - confirmation measurement needed ^{229}Th(n,fission) - confirmation measurement needed ^{227}Th(n,fission) - confirmation measurement needed ^{187}W(n,y)^{188}W - reported value not reliable ^{133}Ba(n,y)^{134}Ba - confirmation measurement needed ^{107}Ag(n,y)^{108}Ag$\rightarrow$^{108}Cd(n, y)^{109}Cd - confirmation measurements needed	**Data for SHE target isotopes production** ^{248}Cm(n,y) low energy resonances ^{249}Bk(n,y) ^{250}Cf (n,y) and ^{250}Cf (n,f) ^{251}Cf(n,y) and ^{251}Cf (n,f) – first resonance	**Data for ^{252}Cf production** ^{245}Cm(n,y) ^{247}Cm(n,y) ^{248}Cm(n,y) ^{249}Bk(n,y) ^{250}Cf(n,g) and ^{250}Cf (n,f) ^{251}Cf(n,g) and ^{251}Cf (n,f) ^{252}Cf(n,X) - resonance near 1eV in particular

3.4 THE REALITY OF AN INSTRUMENT WITH MULTIPLE CAPABILITIES

All of this said, CERBERUS has the potential to become over-subscribed in a short time given its simplicity and flexibility in operation. Much thought will need to be put into understanding the allocation of beam time towards each science goal. Advanced planning will be needed to ensure that alignment of spectroscopy samples is given priority at the beginning of cycles to be sure that all possible samples that may be needed will be ready for mounting at their instruments anytime in the cycle. One hopes that this can be completed in a few weeks or a month of beam time.

Coordinating operations with VISION experiments that would also benefit from the use of BeFAST would be the next priority. Hopefully, those experiments would be as contiguous as possible but there would be some amount of flexibility here provided by the modular nature of the proposed design. Change over between techniques would occur during accelerator maintenance days and good operations planning would allow for a new user to start the day after when neutron production is restored. In the event that a changeover were to take longer, the system would be designed such that the secondary shutter and other shielding is radiologically substantial enough to permit changeover during normal production beam operations at full power.

4. INSTRUMENT DESCRIPTION AND ANTICIPATED PERFORMANCE

The CERBERUS instrument at BL16a of the first target station at SNS utilizes the upstream side of a poisoned and decoupled thermal water moderator. This moderator provides substantial beam brightness at 25 meV (1.8Å) neutron energies with unrivaled energy resolution and instantaneous flux. An unobstructed view of this moderator provides a beam of high energy neutrons to 1MeV and beyond. The front (upstream of the sample position) will have no guide system; only defining apertures, a secondary shutter, bandwidth (BW) chopper, energy filters, and streaming shielding. There will be a beam monitor immediately downstream of the final adjustable aperture to be used for beam normalization. The sample position is at 20 meters, and the design within 50 centimeters of that position will be modular to accommodate the proposed experimental configurations and any others that may arise in the future. Estimates of performance are simulated using the McStas neutron ray-tracing package [1] and analyzed and presented using Python modules NumPy [2] and Matplotlib [3]. Final simulation source code has been loaded into a local repository for further development and refinement of the design [4].

4.1 ALIGNMENT STATION (AS MODE)

The alignment station configuration will utilize slits 1 meter upstream of the sample to define the final beam geometry and position. The sample to be aligned will be mounted on a goniometer that provides full XYZ positioning and orientation capability to simplify the crystal alignment process. Detector coverage will be provided by ^{3}He LPSD tube 8-packs expected to cover 2θ in the range of 30° to 150° on both sides of the scattering sample. In addition, there will be a CCD neutron camera (TOF insensitive) mounted just down steam of the goniometer to provide imaging support of the crystals to be aligned.

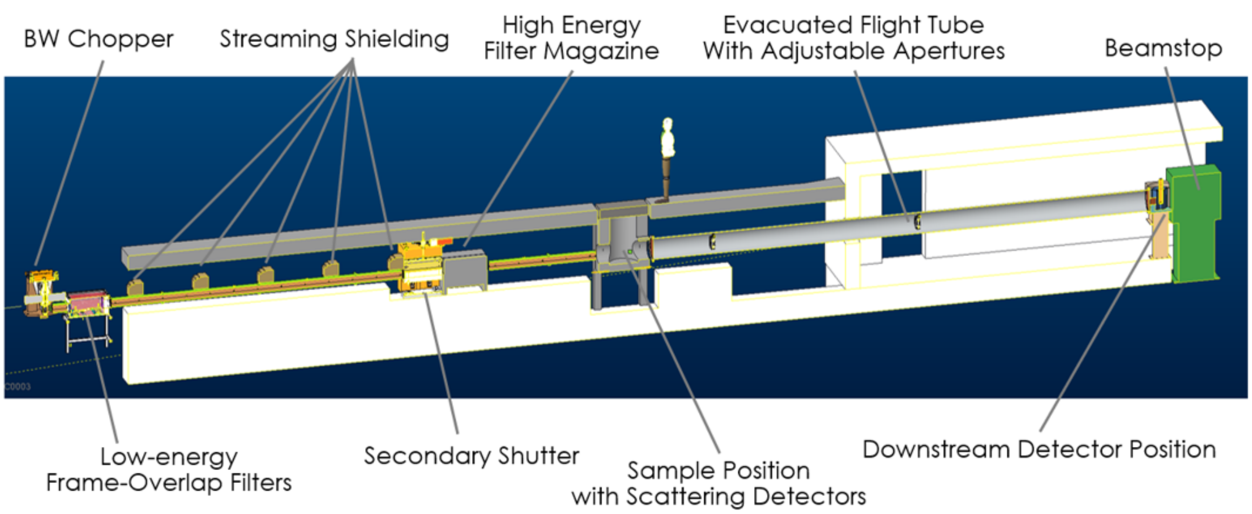

Figure 4. An isometric view of the proposed layout for CERBERUS at BL16a at the SNS-FTS. The neutron beam originates from the left of the view, approximately 8 meters upstream of the bandwidth (BW) chopper. Proposed features include low-energy filters to prevent contamination from prior pulses, streaming shielding to minimize scattered background from both the chopper and the filters, a secondary shutter, a high-energy filter magazine and fully adjustable apertures along the entirety of the flight path to ensure a clean beam phase-space.

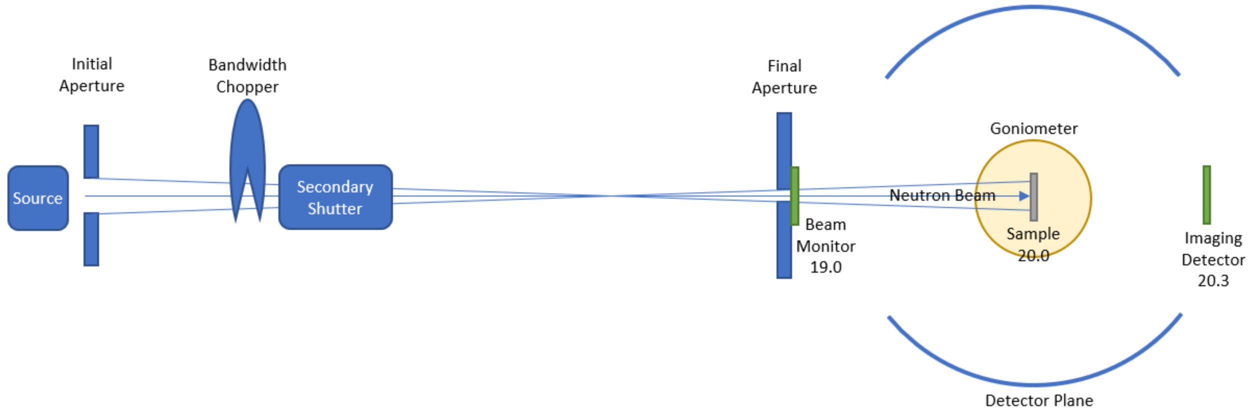

Figure 5. A schematic layout of the Alignment Station (AS) module for CERBERUS. The AS mode will include scattering detectors, a goniometer, and a downstream imaging detector.

In addition to precise vertical alignment by the motor axis on the goniometer, there will also be an elevator system to enable easy access to the goniometer sample mount. This will provide two benefits; first, this will make frequent access to sample position easier for users and secondly, it will permit safe sample access, as components activated by the direct beam will remain in the radiological enclosure. This lowers the dose burden to staff and ensures an additional layer of safety with regards to personnel proximity to the direct beam and components that may have been activated by that beam.

Beam flux in the wavelength range of 0.29Å-2.86Å is 4.18x10^7 neutrons/(cm^2-second) with an available on-sample beam footprint of 3cm wide by 5cm tall. Full-Width at Half-Maximum beam divergence is 0.28° horizontal by 0.34° vertical. Both the position, size, and divergence of the beam are completely adjustable by use of non-fixed initial and final apertures.

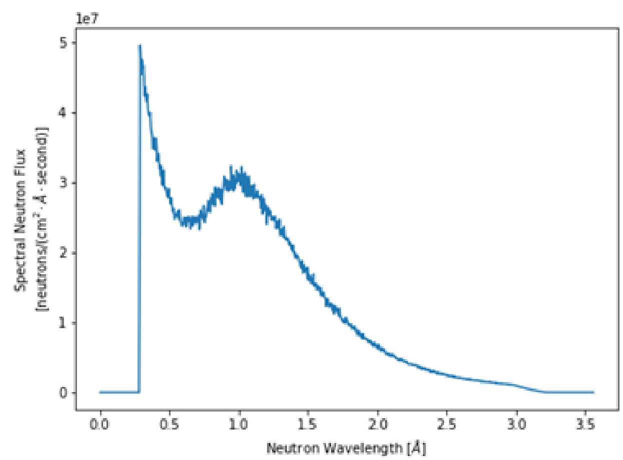

Figure 6. On-sample spectral neutron flux for the Alignment Station configuration. Wavelengths shorter than 0.3Å were not considered relevant to the performance of the AS configuration and were not included in the plot.

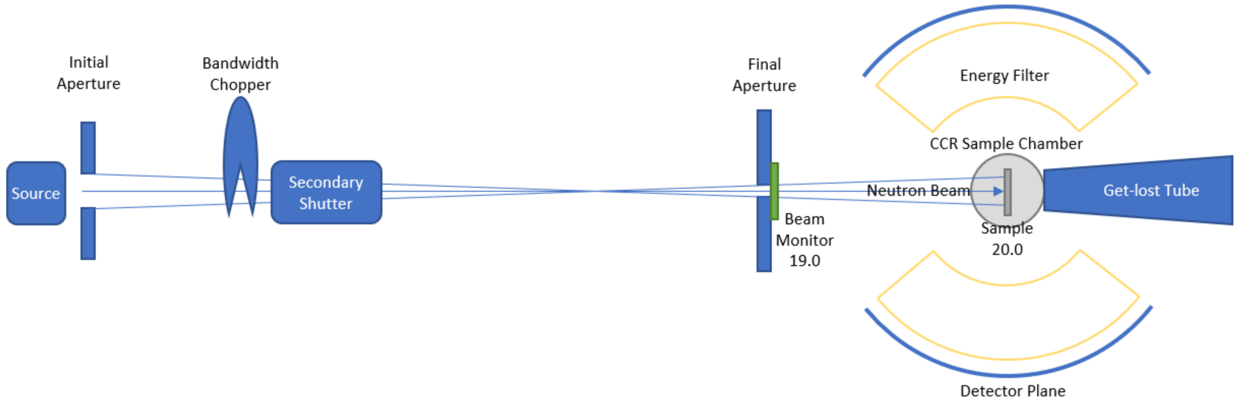

Figure 7. A schematic plan-view layout of the Filter Spectrometer (BeFAST) module for CERBERUS. The BeFAST mode will include scattering detectors, filters, a CCR, and a get-lost tube to minimize background.

4.2 FILTER SPECTROMETER (BeFAST MODE)

The filter spectrometer will also utilize the upstream slits and beam monitor systems to define the final beam geometry and normalize sample scattering. It will utilize the same LPSD tubes proposed for the Alignment Station mode, but include an actively cooled filter material (Beryllium, Graphite, or poly-crystalline Diamond) with built in radial collimation between the sample and those tubes to enable the spectroscopic capability. In addition to the active cooling of the filters, there will be a dedicated CCR for cooling samples down to 4K with precision as good as 0.1K or better. For this system, the neutron camera will not be needed, and could be a potential source of background. Thus, a get-lost tube will be implemented in that location to minimize background from the sample environment and any associated exit windows.

Beam performance is expected to be comparable to the Alignment Station mode, with beam flux between 10-1000 meV 4.18x10^7 neutrons/(cm^2-second), an available beam footprint of 3cm wide by 5cm tall, and FWHM beam divergence is 0.28 degrees horizontal by 0.34 degrees vertical.

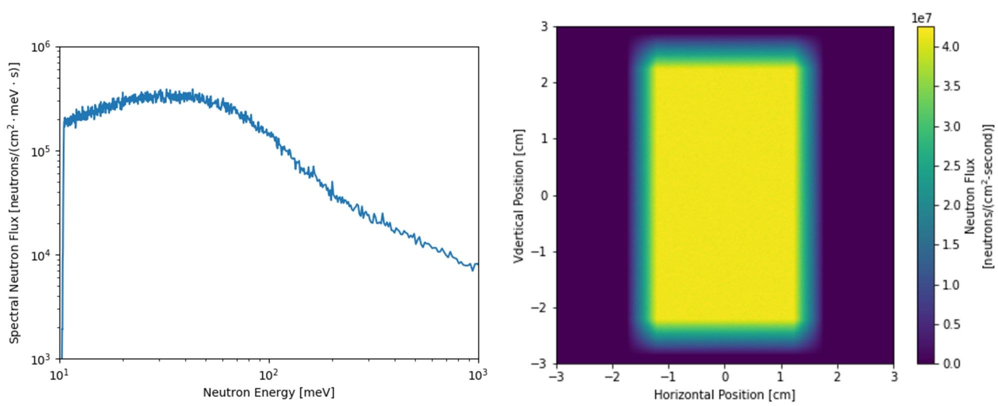

Figure 8. On-sample spectral neutron flux (left) and flux distribution (right) for BeFAST.

4.3 NEUTRON TOTAL CROSS-SECTION SPECTROMETER (XSM MODE)

Support for neutron cross-section measurement will come in two flavors. The first is the loading and changing of a sample series at the 20 meter sample position. There will be a time-of-flight and energy sensitive detector at 31.5 meters that will be used to measure the total attenuation by the material (typically referred to as a transmission measurement) at the sample position. The distance between the sample and the detector will cut down on noise contributions due to scattering effects. There will be adjustable slits and room for supplementary shielding in this area as well. The second option will be a fission-chamber at 31.5 meters to measure the neutron induced fission cross section versus neutron energy. This will be used to measure absorption (fission) cross sections of the material in question. Furthermore, replacing the fission chamber with an ion chamber will permit studies of (n,p) and (n,α) cross-sections, thus contributing yet another measurement capability. This is a technique that was used at the ORELA white neutron source with great success. This, as well as simulated performance estimates can be seen in Figures 9 and 10.

The experimental realization of the neutron transmission method is relatively simple. Fundamentally, all that is needed is a well collimated neutron beam, a sample changer, and a neutron detector. The quantity measured is solely the counts in the neutron detector with sample and without sample, normalized to some neutron production metric. The ratio of the normalized and background corrected count rates from sample in versus sample out gives the transmission.

The width of the SNS proton-beam pulse is approximately 350 ns. This taken in combination with the 31.5 meter flight path length provides a sufficient neutron energy resolution that can be achieved to resolve individual resonances of a cross section. The resolution of the resonances depends on the nuclei under investigation, i.e., on their level density and nuclear structure. SAMMY [5] was used to calculate the anticipated resolution, which includes the contributions from moderator thickness, flight path length and pulse width, seen in Figure 11. Here, the level densities are marked for some isotopes of interest. Note that the resolution of the resonances of a particular nucleus can be hindered by the Doppler effect; meaning that even though the experimental resolution is sufficient it can be hampered by the movement of the nucleus. By using a cryogenic device to cool the sample, the Doppler broadening can be reduced.

Depending on the neutron energy of interest either a more efficient ^{6}Li loaded glass scintillator for energies from thermal to about 200 keV is used or a fast plastic scintillator which is more efficient for neutron energies above 100 keV. It would be ideal to have different neutron detectors with different thicknesses, to accommodate efficiency and count rate problems. The samples are usually cycled through the beam with a fixed number of pulses per sample. This helps to reduce systematic effects from changes of detector

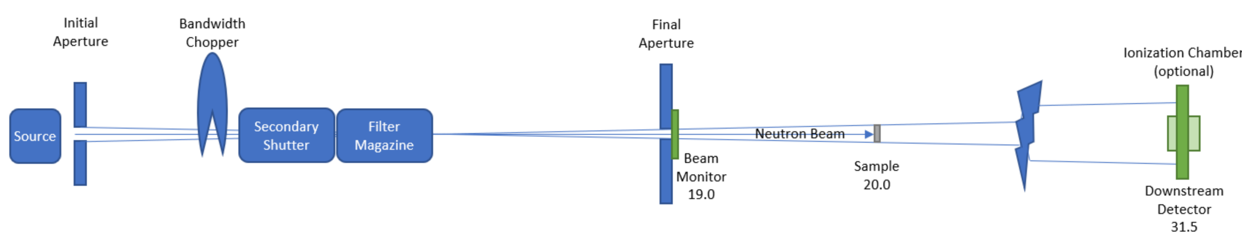

Figure 9. A schematic plan-view layout of the Cross Section Measurement (XSM) module for CERBERUS. The XSM mode will include a magazine of energy filters, support for an Ionization Chamber, a sample loader and changer, and a downstream detector used to resolve attenuation by the sample and upstream filters.

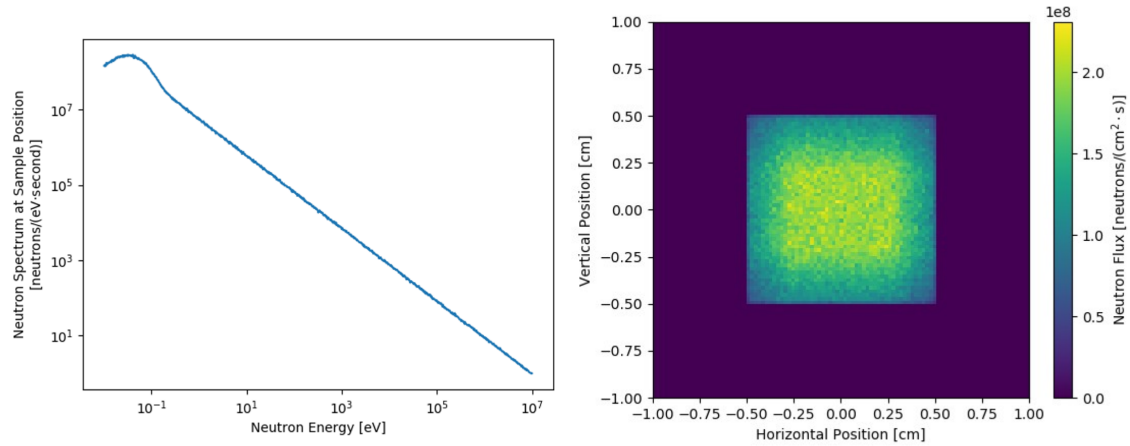

Figure 10. Plots describing the CERBERUS beam character while operating in XSM mode. (Left) The time-averaged neutron spectrum anticipated at the sample position for a 1cm x 1cm beam footprint. (Right) The neutron flux distribution under the same conditions.

efficiencies and beam intensities over time. The instantaneous neutron spectral intensity will be important to ensure pulse pile-up issues are not encountered at the highest of neutron energies. This will directly inform the required detector efficiency for a certain energy regime.

The biggest challenge for transmission experiments using a small sample is the sample preparation and the collimation of neutron beam in combination with a sample changer. Transmission samples should be uniform in thickness and homogeneous; small samples will be in the range of µg to mg and thus fabrication will be a challenge. As the diameter will be very small, in the 1mm or below range, the collimation and alignment with the sample changer will be critical. Using modern stepping motors to control the sample changer, a precision of less than one micron can be achieved yielding a precise alignment between sample and collimator. The diameter of the collimator needs to be smaller than the sample diameter and sufficient shielding around the collimators is required to block the scattered neutrons from reaching the neutron detector. These developments will be a critical part of a fully developed design.

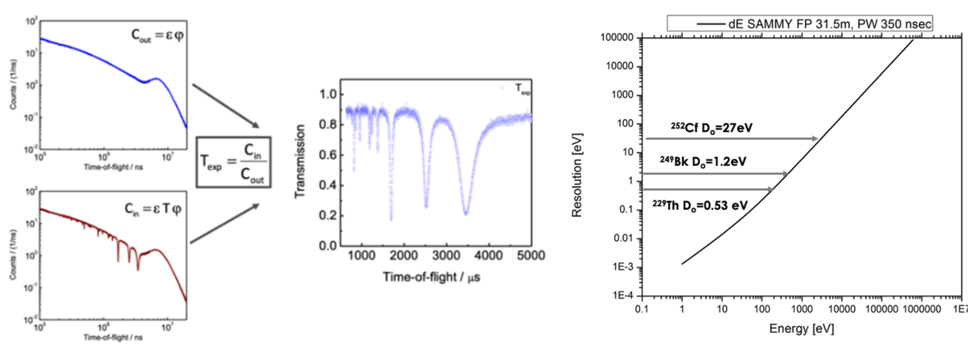

Figure 11. Plots describing the anticipated data reduction and resolution performance in the XSM mode of CERBERUS. (Left) Basic data reduction methodology for transmission measurements. (Right) An estimate of the energy resolution for various isotope resonances of interest, taking into account instrument effects based on the anticipated CERBERUS geometry.

5. COST ESTIMATE AND INITIAL RADIOLOGICAL SIMULATION

The estimation of project cost is based on recent procurement data, raw materials costs, and instrument engineering tacit knowledge. The estimate provided is only a rough estimate and may not reflect very recent changes in costs due to price increases in labor, materials, or other subcontracted procurements to be charged, and can be found in Table 2.

Shielding material and fabrication costs were determined using first order radiological calculations and simulations using MCNP 6.2 [6]. Those calculations will need further refining in the next stage of design and development but are suitable for initial beam stop and instrument enclosure cost estimates. Contour plots describing the dose rates at given shielding thicknesses are seen in Figures 13 and 14 for both gamma and neutron exposure levels.

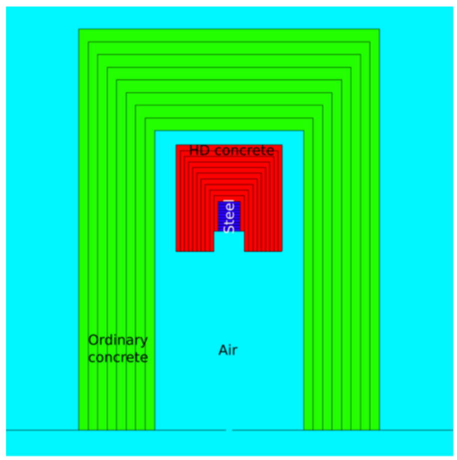

Figure 12. The simulated shielding layout near the beam stop for the first order MCNP radiological calculations. These are rough calculations used to understand the potential materials and fabrication costs associated with the beam stop design.

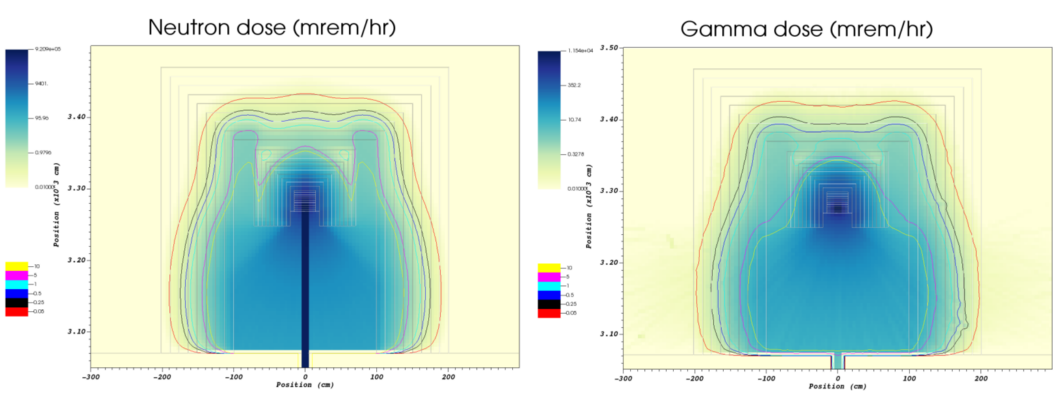

Figure 13. MCNP calculated dose rates in and around the beam stop.
The black contour line is the 0.25 mrem/hr dose rate boundary.

Table 2. A table with the cost estimation of parts and assemblies for the proposed CERBERUS Instrument.

Top Level Assembly/Part	*Qty*	*Total*
Utilities & Infrastructure		**$ 28,320.00**
New Sprinkler Piping	1	$2,500.00
New Vacuum Piping	1	$2,500.00
HVAC Unit	1	$8,320.00
House Compressed Air Interface and Runs	1	$5,000.00
House SCW interface and Runs	1	$5,000.00
House Nitrogen interface and Runs	1	$5,000.00
Technical Components		**$ 2,708,500.00**
Beam Tube Assembly	1	$208,000.00
Secondary Shutter	1	$150,000.00
Sample Stand - Base Structure (Elevator)	1	$115,000.00
Ancillary Equipment	1	$11,500.00
Adjustable Beam Defining Slits	4	$160,000.00
8-pack LPSD with 8mm dia x 30cm long 3He tubes	1	$875,000.00
Sample Cryostat	1	$155,000.00
Beryllium Filter Housing with CCR	2	$65,000.00
Beam Monitor	1	$10,000.00
BW Chopper	1	$400,000.00
High Energy Filter Magazine	1	$65,000.00
Wavelength Filter V-cavity	2	$130,000.00
Sample Goniometer	1	$100,000.00
Downstream Streaming Composite Shielding Package	900lbs	$18,000.00
Upstream Streaming Composite Shielding Package	900lbs	$18,000.00
Neutron CCD Neutron Camera	1	$8,000.00
Downstream Detector	1	$200,000.00
Beamstop	1	$20,000.00
Shielding		**$ 117,088.66**
SD Concrete Delivered	71 cu yds	$14,188.96
HD Concrete Formed Roof - Steel Cased	27 cu yds	$102,899.70
PPS		**$ 65,660.00**
PPS / ODH Hardware		$50,000.00
Smoke Detector		$1,000.00
Sprinkler Reconfiguration		$14,660.00
Electrical / DAS / Controls		**$ 170,600.00**
Field Cabling	1	$2,600.00
Data Analysis Workstation	1	$25,000.00
Desktop Computer	1	$15,000.00
8-Axis MC Cabinet	3	$45,000.00
Cables/Electrical/Encoder Support	1	$10,000.00
Cable Management	1	$4,000.00
AC Power - Wall/Cabinets	1	$9,000.00
Half Rack	1	$4,000.00
Encoders / Motors / Limit Switches	8	$32,000.00
FEM	3	$12,000.00
DSP	1	$4,000.00
ODB	2	$8,000.00
Estimate Grand Total		***$ 3,090,168.66***

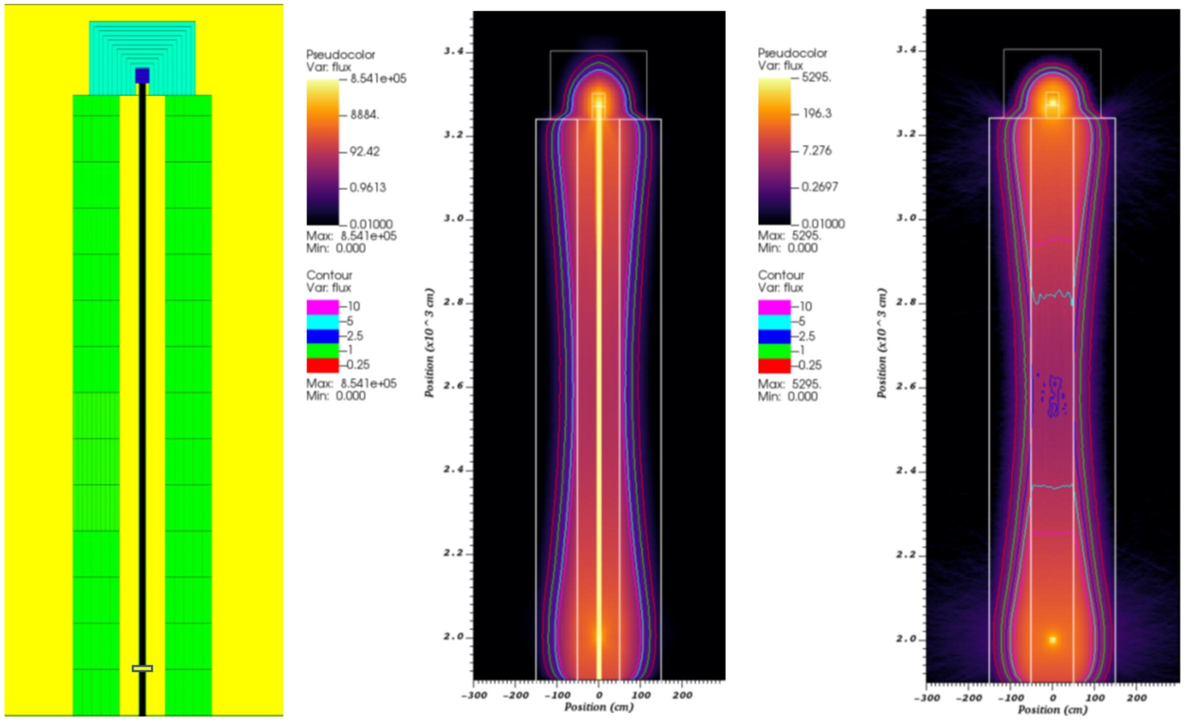

Figure 14. MCNP Calculated dose rates from the sample position to the beam stop. (Left) A MCNP geometry representing a 1cm steel plate at the sample position within a SD concrete tunnel, a HD beamstop case and steel beamstop. (Middle) Simulated neutron pseudocolor-flux and dose-rate contour levels. (Right) Simulated gamma pseudocolor-flux and dose-rate contour levels.

6. CONCLUSION AND ACKNOWLEDGEMENTS

The proposed instrument CERBERUS will provide an infinitely better capability than that which is currently delivered by the open beam port at 16a of the FTS at SNS. The preliminary beam design, radiological simulations and cost estimates contained herein are only a starting point in the larger project plan that would be required to realize such an instrument investment. There are letters of support located in the Appendix A that emphasize the real impact that such an instrument capability would have if it were to become a reality. One hopes that the developments and analysis presented are suitable to continue refining the design and take the next steps to further enhance the neutron science contribution of ORNL. The authors would like to acknowledge the exceptional work of David Conner for cost estimates and preliminary design concepts, Kyle Grammer for providing radiological calculations and shielding optimizations, and Georg Ehlers for discussions and guidance during the conceptual development process.

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APPENDIX

A EXTERNAL LETTERS OF SUPPORT

Find in the next pages three letters of support from respected members of the user community that would benefit from the CERBERUS scattering instrument. Any reference made to the "MSAS Instrument" or the like implies the proposed CERBERUS instrument.

THE UNIVERSITY OF
TENNESSEE
KNOXVILLE

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September 23, 2022

Dear Dr. Guber,

We want to welcome and express our strong support for the construction of the ORNL initiative to construct a Multi-purpose Spectrometer and Alignment Station (MSAS) at SNS BL16. For decades, the experimental nuclear physics community collaborated with ORNL researchers in leading cutting-edge science in fundamental and applied nuclear physics. The interactions with the ORNL scientists and the use of ORNL facilities have benefitted UTK faculty and students, and we look forward to being involved in this project. We are very interested in exploiting the discovery potential of this new experimental system to expand our science program. The access to a local facility will also enable more opportunities for our students to interact with ORNL scientists and acquire more hands-on experience with nuclear instrumentation.

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Kate Jones,
Professor of Physics and APS Fellow
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401 Nielsen Physics Building
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Rensselaer | DEPARTMENT OF MECHANICAL, AEROSPACE, AND NUCLEAR ENGINEERING

October 20, 2022

Dear Dr. Brown

It is my pleasure to write this letter to support the proposal titled "MSAS: Multi-purpose Spectrometer and Alignment Station"

I am a Nuclear Engineering professor at Rensselaer Polytechnic Institute (RPI), holds the Edward E. Hood Jr. Endowed Chair in Nuclear Engineering, Director of the Gaerttner LINAC Center, and the Director of the Nuclear Engineering Program. I served as a member of RPI's university wide promotion and tenure committee, and as President and Chair of the Faculty Senate. I have been serving on the US Cross Section Evaluation Group (CSEWG) since 2007 as chair of the measurement committee; I am also a member of the Nuclear Data Advisory Group (NDAG) for the DOE Nuclear Criticality Safety Program (NCSP) since 2008, and ANS fellow.

As evident from the paragraph above, my interest is in nuclear data, particularly in cross-section measurements. The proposal includes Neutron Induced Cross-section Station that will enable high accuracy cross section measurements at SNS. The unique high flux and relatively short pulse enable measurements in the sub-thermal, thermal, and low eV energy range. This is extremely important to provide data to variety of applications. The proposal provides example of medical isotope production calculation where such cross sections are needed. Currently also U-235 which is used in many applications does not have good, measured data in the sub-thermal region which influences reactor calculations. Such a beamline will diversify the activity as SNS and provide an important contribution to the nuclear engineering community that needs more accurate data.

Supplementing VISION with BeFAST can also help in development of thermal scattering laws for moderators including those used for nuclear reactors and future neutron scattering applications (such as SNS). Previously we used VISION data for development validation of atomistic calculations that are the basis for thermal scattering evaluations used in the nuclear application and the nuclear energy industry.

At RPI we have a LINAC that is currently being upgraded to a higher power and neutron production and is used for cross section measurements. It is one of very few facilities that train the future manpower that the DOE needs, adding the new beam line as SNS will also help SNS train future scientist in performance of stat of the art nuclear data measurements.

Increasing the portfolio of SNS and thus attracting other users increases the visibility and importance of the facility to advancement of science in multiple directions. I thus fully support this new beam line and hope this proposal will be unded.

Sincerely,

Rensselaer Polytechnic Institute
110 8th Street | Troy, NY 12180-3590 USA

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

October 13, 2022

Subject: SNS experiments

Dear Dr. Guber,

On behalf of the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) I want to express my strong support to the ORNL initiative to construct a Multi-purpose Spectrometer and Alignment Station (MSAS) at the ORNL Spallation Neutron Source (SNS) BL16. As explained in the proposal, the proposed beamline is well suited to perform Nuclear Data (ND) experiments on radioactive samples which are of great need for practical applications. As of today, there are very little information on data for radioactive samples that can be used for producing data evaluation for inclusion in evaluated nuclear data libraries. In addition to the measured data the associate uncertainties are very important for application. As a French entity IRSN collaborates for almost a decade with ORNL thru the Nuclear Criticality Safety Program (NCSP) on the field of ND and related experiments for application in criticality safety and reactor applications. An example is the IRSN/ORNL collaboration on measuring and evaluation of thermal neutron scattering kernel experiments carried out at SNS. The prospect of obtaining nuclear data for radioactive samples will be very useful in our criticality safety applications. I want to emphasize out full support as we are in need for better data for those isotopes for our M&S calculations.

Yours sincerely,

Luiz Carlos Leal

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