ORNL/TM-2020/1568

# Conceptual Design Report
# A Replacement Cold Neutron Guide System for HFIR


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OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

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Neutron Sciences Directorate

# CONCEPTUAL DESIGN REPORT
# A REPLACEMENT COLD NEUTRON GUIDE SYSTEM FOR HFIR

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## ABBREVIATIONS, ACRONYMS, AND INITIALISMS

| | |
|---|---|
| BES | DOE Office of Basic Energy Sciences |
| Bio-SANS | Biological SANS (existing HFIR instrument) |
| C-TAX | Cold Triple-Axis Spectrometer (existing HFIR instrument) |
| DOE | US Department of Energy |
| FOV | field of view |
| FWHM | full width at half maximum |
| GP-SANS | General Purpose SANS (existing HFIR instrument) |
| HFIR | High Flux Isotope Reactor |
| HWHM | half width at half maximum |
| IMAGINE | Laue Diffractometer (existing HFIR instrument) |
| IMAGING | Neutron Imaging Facility (existing HFIR instrument) |
| Larmor | proposed test and development instrument to be located temporarily on NB-2 |
| MANTA | Multi-Analyzer Triple-Axis Spectrometer (proposed new instrument) |
| NScD | Neutron Sciences Directorate |
| NVS | neutron velocity selector |
| ORNL | Oak Ridge National Laboratory |
| SANS | small-angle neutron scattering |
| SNS | Spallation Neutron Source |

**ABSTRACT**

The design of a replacement cold neutron guide system for the High Flux Isotope Reactor (HFIR) is presented. The proposed six-channel design uses the latest technologies and is optimally designed to account for operational and site constraints. These include the design of the cold source and the beam tube, the size and shape of the penetrations in the reactor confinement boundary, and the shape and orientation of the guide hall. The existing user instruments are a macromolecular diffractometer (IMAGINE), an IMAGING station, two small-angle neutron scattering (SANS) instruments (Bio-SANS and GP-SANS), and a cold triple-axis spectrometer (C-TAX). These instruments will all be reinstalled at end-of-guide positions with improved performance, and a position for a new high-performance neutron spin echo instrument will be created. The proposed guide design requires an extension to the guide hall toward the south.

The calculated flux gain for a typical experiment is between a factor of 1.3 and 3 for all instruments, with the exception of the C-TAX instrument, which stands to gain a factor of >30 in flux at the sample. The new guide system will also offer additional performance gains, such as an increase in Q-range on Bio-SANS. The stated performance gains do not take into account any potential performance gains resulting from renewal and realignment of the guide system.

The design of the guide system in the common sections up to about 25 m from the source is considered to be complete and ready for engineering design, while the designs of the instrument-specific guides are in some cases still a work in progress. The present report describes the current status of those designs.

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# 1. INTRODUCTION

The Neutron Sciences Directorate (NScD) at Oak Ridge National Laboratory (ORNL) operates two neutron sources—the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS)—for the US Department of Energy (DOE) Office of Science, Basic Energy Sciences (BES). HFIR is an 85 MW reactor that provides one of the highest continuous neutron fluxes of any research reactor in the world. HFIR currently supports a vibrant neutron scattering user program across 12 instruments along with 4 development beamlines.

Planning has begun for a replacement of the reactor’s permanent beryllium reflector in 2024, which will require an extended outage of some 9–12 months. The reflector changeout is driven by operational requirements of the reactor; and as part of this work, the HFIR beam tubes and the cold source will also be replaced. The outage presents a rare opportunity to refurbish the network of cold neutron guides to best serve the proposed suite of neutron scattering instruments in the HFIR Cold Guide Hall from 2025 and into the future. A number of options for the replacement guide system have been conceptually explored through performance evaluations based on Monte Carlo methods. This technical report documents the conclusions of these studies. The neutron-optical design of the front-end part of the guide system is complete and ready for detailed engineering design and feasibility studies. This design includes sections of the network in which the guides are physically close to each other and share common vacuum housing and shielding, up to about 25 m from the cold source. Downstream of this location, the neutron-optical design is still being refined.

## 1.1 HFIR HISTORY

HFIR is a beryllium-reflected, light water–cooled and moderated flux-trap type reactor that uses highly enriched uranium-235 as the fuel. The reactor first went critical in 1965 with the highest continuous neutron flux in the United States both in the core and the beam tubes and retains this title after completing its 487$^{th}$ fuel cycle in May 2020. Today HFIR retains its original mission and fundamental focus on isotope research and production; however, its primary purpose has evolved to support neutron scattering research.

Following the last beryllium reflector replacement in 2000, a series of major upgrades were completed, including installation of the hydrogen cold source in the HB-4 beam tube, construction of the present guide hall, and installation of the current cold neutron guide network. HFIR restarted in 2001, and the neutron scattering User Program, with its particular focus on cold neutrons, has emerged since 2007. One measure of the success of this program development is that the cold neutron guide hall at HFIR is now at capacity. The beryllium-reflector replacement thus provides an opportunity to reoptimize the instrument suite.

## 1.2 OVERALL GOALS

The overall goals and guiding principles behind the design of the replacement guide network may be summarized as follows:

- Capitalize fully on technological improvements in neutron optics designs and materials made since the present guide system was designed and installed.

- Reconfigure the network to afford improved performance and additional end-station locations.

- Follow, to the extent possible, guidance from the ORNL Neutron Sciences Instrument Advisory Board [1] (also see Appendix A) regarding upgrading the cold neutron delivery system
  - to develop a national roadmap for neutron spin echo
  - to develop a modern guide and the primary spectrometer for a new cold triple-axis spectrometer
  - to ensure the new cold guide system should not degrade the performance of the cold imaging station and should enhance it if possible

The user community, instrument suite reviews, and NScD staff members have all contributed to the decision-making process; and, understandably, there is a strong desire not to lose any existing capabilities as a result of the beryllium reflector replacement.

## 1.3 SITE CONSTRAINTS

As stated earlier, the beryllium reflector replacement provides a rare opportunity to reoptimize the cold neutron scattering instrument suite. This optimization process, however, is bounded by a number of physical constraints imposed by the site and the reactor facility.

The time-averaged brightness of the cold source at HFIR, at 5 Å, exceeds that of the SNS First Target Station coupled moderators by about an order of magnitude, and that of the currently planned SNS Second Target Station moderators by about a factor of two. HFIR thus provides opportunities for world-class cold neutron instrumentation. However, the performance of the cold neutron instruments is compromised by the beam extraction arrangement, in which a rather small (softball-size) cold source is viewed by a guide system in the existing installation starting at approximately 5 m. The design of the new guide network will seek to reduce this distance in an effort to improve the situation, but the cold guides will still be significantly under-illuminated for many applications. The situation is compounded further by two critically important design features of the HB-4 beam tube:

- Load lines for the cold source which must be routed inside the HB-4 beam tube, limit the view port to the moderator.

- Inside the downstream portion of the HB-4 beam tube is an internal collimator, which serves several safety-related functions relevant to reactor operations and significantly restricts the solid angle within which instruments can view the source.

A second site constraint comes from the orientation of the Cold Guide Hall relative to the HB-4 beam tube, as shown in Figure 1. When the guide hall was first constructed as a laydown space for equipment, its footprint was bounded by the adjacent buildings that could not feasibly be reconfigured (Figure 1). As a consequence, the beam tube centerline enters the guide hall east of the center of the north wall and is pointed toward the east side of the building. Although the guide hall cannot be extended to the east, it is feasible to extend it to the south.

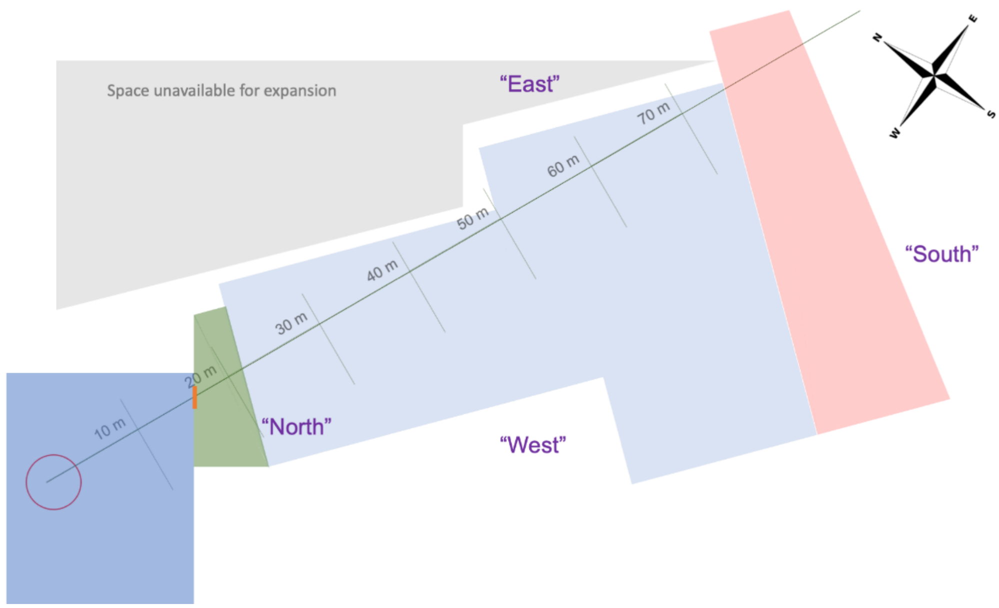



**Figure 1. Overall layout of the neutron guide hall relative to the HB-4 beam tube center line.** Red circle: reactor pool; green line: HB-4 beam tube center line; dark blue: (part of the) reactor confinement building; light green: transition building; orange line: bulkhead wall with tight constraints on the beamline locations; light blue: existing guide hall; light red: proposed expansion of the guide hall; gray: space unavailable for expansion.

The third major constraint comes from the pass-through in the bulkhead wall between the beam room and the transition building (shown in light green in Figure 1), which forms part of the confinement boundary of the reactor building. Unfortunately, the rectangular opening in this wall is centered somewhat below the beam axis, defined as the straight line connecting the center of the cold source and the center of the collimator opening in the beam tube. The current guides thus traverse the bulkhead well above its centerline, impacting on the available guide height. Modifications to the bulkhead wall have not been pursued, as they would impact the safety-related functions relevant to reactor operations.

## 2. OPTIMIZATION PROCESS FOR THE GUIDE SYSTEM DESIGN

To understand the optimization process requires an overview of the current situation. The cold source is located at the tip of a horizontal beam tube that penetrates the beryllium reflector and views the reactor core tangentially. The tube is schematically shown in Figure 2 below.

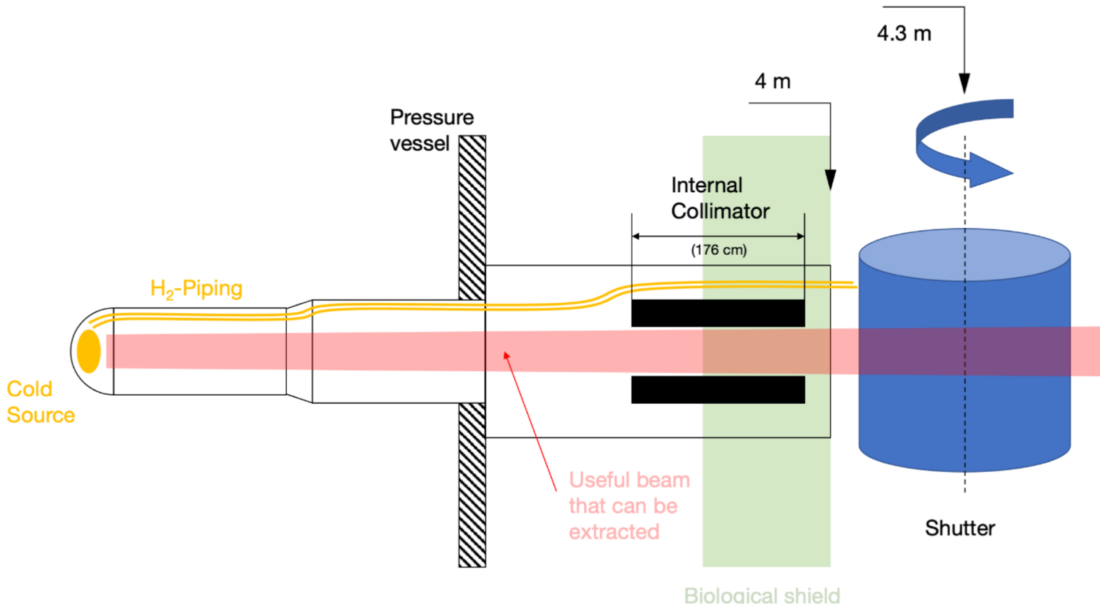



**Figure 2. The HB-4 beam tube, with the cold source highlighted at its tip.** Downstream of the tube is the primary shutter for all cold beams. The downstream end of the tube as shown is at approximately 4 meters distance from the cold moderator surface.

Following the guiding principles set out in Section 1.2, optimization of the new guide configuration has four main drivers:

1. Add a new spin echo neutron spectrometer to the cold neutron instrument suite.

2. Increase the number of guides from four to six so that every instrument can be on an end-guide position.

3. Improve instrument performance where possible.

4. Ensure that after the guide reconfiguration, every instrument performs at least as well as it currently does.

Given NScD's desire not to lose any existing capabilities (see Figure 3) following installation of the new guide network, the following is the long-term vision for the cold neutron instrument suite:

| | |
|---|---|
| NB-1: | the IMAGINE quasi-Laue macro molecular diffractometer |
| NB-2A: | a sample alignment station |
| NB-2B: | the neutron spin echo spectrometer |
| NB-3: | Bio-SANS, the biological small-angle neutron scattering (SANS) instrument |
| NB-4: | IMAGING, the cold neutron imaging instrument |

NB-5: GP-SANS, the general-purpose SANS instrument
NB-6: MANTA, the multi-analyzer triple-axis spectrometer

This suite replicates the current suite with the exception of the multi-analyzer triple axis instrument (currently operating there is a cold triple-axis instrument of a traditional design). The spin echo instrument is the only net addition to the instrument suite.

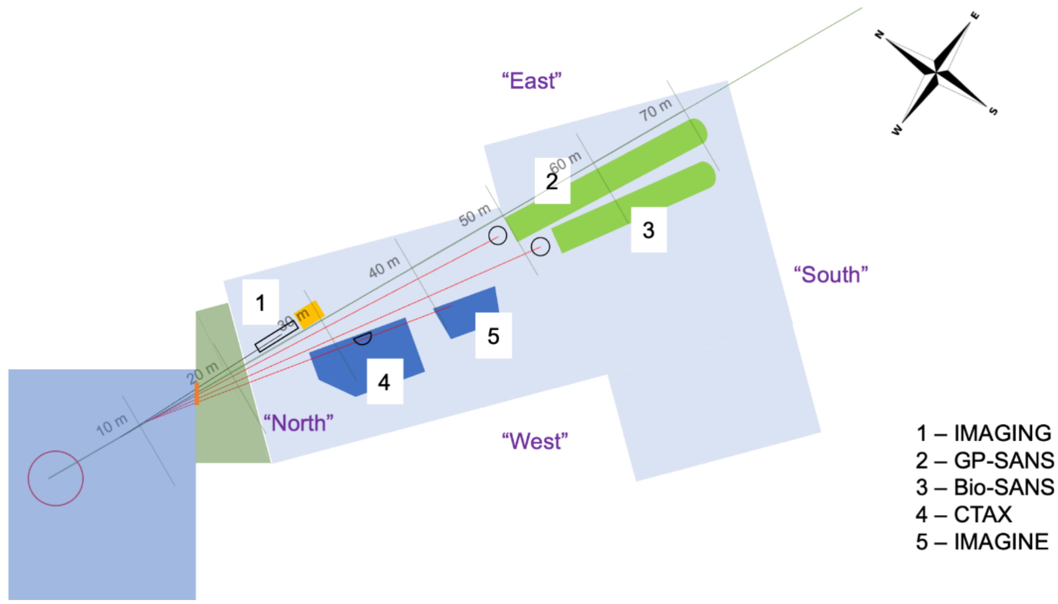



**Figure 3. The current instrument suite as of early 2020.** This shows only the instruments in the user program. Not shown are a test beamline for detector development, a sample alignment station, and a neutron optics test beamline.

The optimization effort was divided into three successive tasks, primarily because the resources were not available to perform a simultaneous optimization across the full set of guide parameters for all instruments. This simplification is justified given the tight physical constraints imposed by the guide hall (see Section 1.3). The three tasks are

1) Partition the viewable solid angle of the HB-4 cold source according to the requirements and constraints for the suite of instruments (covered in Section 4.1).

2) Optimize the guide/instrument layout in the guide hall (described further below in this section).

3) Optimize the individual guides to transport the phase space volume needed by each instrument (covered in Section 4).

For the first task, the most significant constraint is the beam-defining collimator integrated into the HB-4 beam tube. This collimator serves several safety related functions relevant to reactor operations. The instrument design team worked extensively with the reactor engineers to obtain the largest solid angle possible through the internal beam tube collimator. That effort is detailed in Section 4.1.

A second constraint for Task 1 is the orientation of the Cold Guide Hall relative to the HB-4 beam tube (Figure 3 and Figure 4). The reason for the current orientation is that the location of the guide hall was itself constrained by the adjacent buildings that could not be readily reconfigured. The beam tube centerline enters the guide hall east of the center of the north wall and is pointed toward the east side of the building. In addition, all guides are curved to suppress instrument background by avoiding line-of-sight for fast neutrons and primary gammas exiting the HB-4 beam tube and entering the Cold Guide Hall. The result is that the triple-axis instrument needs to occupy the area between the beam tube centerline and the east wall of the guide hall, and there is no room for any other instruments on the east side of the beam tube centerline. This means that the NB-6 guide curves to the east, and the other five guides all curve to the west to avoid line of sight (Figure 4 and Figure 5). The triple-axis instrument can receive the full height of the beam passing through the east side integrated beam tube collimator.


**Figure 4. The proposed new guide hall layout.**

Further constraints for Task 1 derive from the individual instruments. For example, GP-SANS in its current configuration sits in a trench on the guide hall floor because the radius of its detector vessel is larger than the height of the beam at the sample position; hence, the vessel is recessed into the floor. Another example is the Bio-SANS beamline, which is built on a 0.5° incline. Although this incline puts the bottom of the Bio-SANS detector vessel above the floor, it is preferable to avoid changing the angle of the incline for optimized beam transport. The overall elevation of the Bio-SANS detector vessel can be increased should it be decided to increase the length of the instrument.

Task 2 follows from Task 1. We considered various ways in which the instruments could be arranged within the guide hall and simulated the neutron transport to see how well the phase space requirements for each instrument could be met for each configuration (Figure 5). First, NB-5 (GP-SANS) was placed in the guide hall, since its location is constrained by the trench in the floor. Moving GP-SANS out of the trench (sideways) would mean a major additional technical complication, with no improvement to instrument performance, so this option was not considered. The desired wavelength band is 4 Å to 20 Å, and the beam divergence at the sample is controlled in the usual way for a SANS instrument—by selecting and translating individual guide sections in the beam flight path between the entrance aperture and the sample position. The current GP-SANS uses an optical filter to deflect the beam as well as eliminate neurons with wavelengths too short to be useful on this beamline. Changing to a conventional curved guide was considered, but it would require a doubly curved guide to both eliminate line-of-sight from the beam tube into the guide hall and align the detector vessel with the existing trench. The gain from using a curved guide was less than 5% at 4 Å and negligible above 6 Å, and the short wavelengths that the optical filter effectively removes would have to be dealt with. It is possible to move the GP-SANS detector vessel further away (along the trench) to increase the distance between MANTA and the GP-SANS velocity selector. The greater distance would avoid problems with the use of high-power magnets on MANTA and provide more space around the GP-SANS sample area. The GP-SANS beamline is already well optimized for the HB-4 cold source geometry, so only a modest gain could be realized.

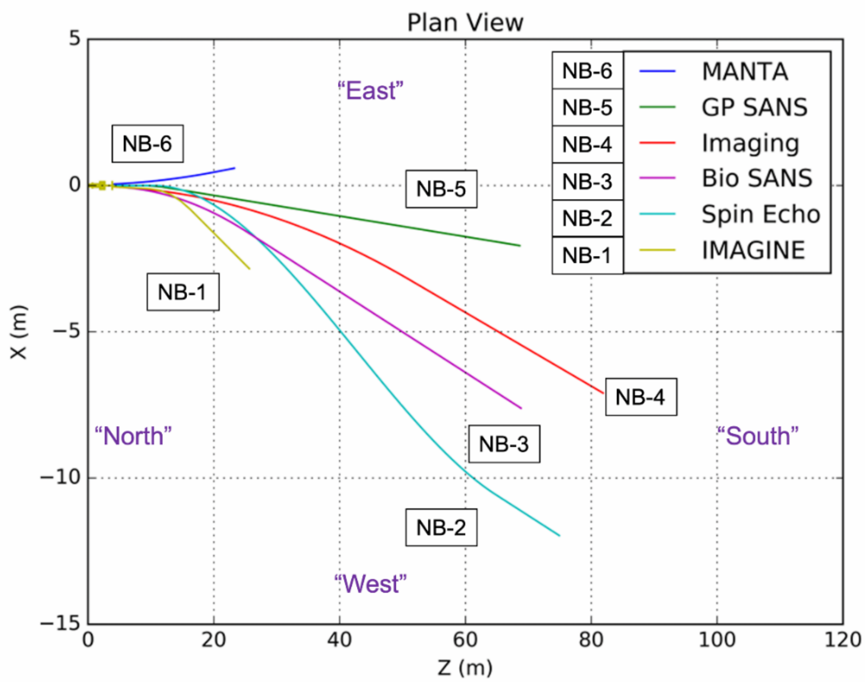



**Figure 5. Plan view of the proposed new guide network.**

Next, NB-6 (MANTA) was placed on the east side of the HB-4 beam tube centerline with the minimum curvature needed to eliminate line-of-sight from the HB-4 beam tube into the guide hall. Using the minimum curvature allows the best transport of short-wavelength neutrons and the most floor space for the instrument. The phase space requirements for MANTA are an $E_i$ of up to 25 meV and enough horizontal and vertical divergence to match the acceptance of a doubly focusing highly oriented pyrolytic graphite monochromator. The NB-6 guide must also allow enough space for a velocity selector and the optical components needed for a virtual source. Details of the final optimization of MANTA are presented in Section 4.

The IMAGING beamline currently occupies the space that MANTA will use on the new guide network configuration (Figure 5 and Figure 6). In this location, the current IMAGING instrument has useful neutron flux down to 1.8 Å. This beamline also needs as smooth a phase space volume as possible, with minimal phase space folding, since structure in the phase space gives rise to artifacts in the final image. To get good short-wavelength transport, the curvature of the new NB-4 guide should be as small as possible. The option of bringing NB-4 to the east of the HB-4 beam tube centerline next to the NB-6 guide was examined closely. It was decided that the performance cost to NB-6 due to the space requirements of the MANTA monochromator was too severe to justify this option. The curvature of NB-6 would have to be increased by more than 0.5°, which would lower the transport efficiency of the shorter-wavelength neutrons and reduce the available floor space, which is already very tight. For the reasons mentioned above, NB-5 (GP-SANS) occupies the minimum curvature position on the west side of the HB-4 centerline. The best option for NB-4 is to move Bio-SANS about 2.5 m to the west to make room for NB-4 to pass between the two SANS detector vessels in the new configuration. It would not be possible to improve the performance of the IMAGING instrument by positioning it on the west side of the current Bio-SANS, because of the amount of curvature in the guide that would be required (greater than 9°). Moving the IMAGING beamline between the two SANS detector vessels requires that the south end of the guide hall be extended by about 5 m.

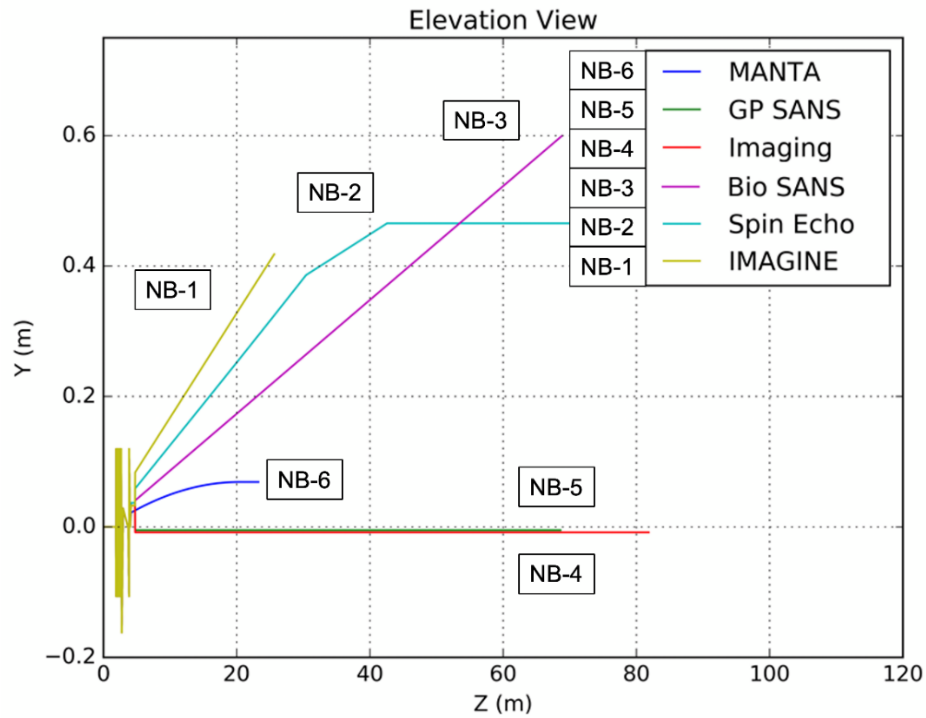



**Figure 6. Elevation view of the proposed new guide network.** The reason that most beams point upward is detailed in Section 4.1.

The present configuration of NB-3 (Bio-SANS) uses a double-bounce optical filter similar to the one used for GP-SANS to achieve a bend of 6°. For the IMAGING guide, NB-4, to fit between the two SANS detector vessels, NB-3 must be bent by at least 9.1° relative to the HB-4 beam tube centerline. With such a large curvature, a conventional curved guide would be expected to clearly outperform an optical filter in a wavelength range where SANS mostly operates (4–10 Å). This was confirmed by simulation.

The NB-2 guide is optimized to transport mostly long-wavelength neutrons, 8 Å and longer. This is the wavelength range required by the spin echo instrument that will eventually be constructed there. In the short term, a Larmor test and development instrument (which will also use long-wavelength neutrons) will use the NB-2 beam. Therefore, the NB-2 guide can be positioned west of the Bio-SANS detector vessel with little loss in performance. The optimization process was also the same for NB-4, but with the relaxed phase space requirements.

Beamline NB-1, which supplies neutrons to the IMAGINE macromolecular diffractometer, has the greatest curvature of 12.7°. It uses a pair of band pass mirrors to select the wavelength band and an ellipsoidal mirror or nested Kirkpatrick-Baez mirror to image the entrance slit onto the sample position with a magnification of 0.1. Because the instrument operates with very small divergence on sample, 0.2° full width at half maximum (FWHM) horizontally and vertically, the beam can be transported to the sample despite the strong curvature of the beam.

Monte Carlo calculations of the neutron transport were made with McStas [2] using the “Source_gen” component. This is a highly customizable McStas component that can be used to accurately model a well-characterized neutron source. This component was used to replicate the neutron spectrum emitted from the cold source in HB-4, informed mainly by a time-of-flight measurement of the source brightness [3] during its commissioning in 2007 (Figure 7). The measurement used a chopper to resolve the cold neutron spectrum via time-of-flight and a series of precision inline apertures in front of a fission chamber counter in direct view of the source. This measurement setup was also simulated in McStas to quantify the actual optical throughput (or acceptance) of the system and determine a precise brightness spectrum. The result was a suitable fit of a triple Maxwell-Boltzmann distribution to the measurement and a set of precisely defined parameters to use in future simulations of instrumentation located in the HFIR Cold Guide Hall. As a result, we have confidence that we can produce absolute flux numbers (at the sample position of an instrument) with good accuracy using the McStas models.

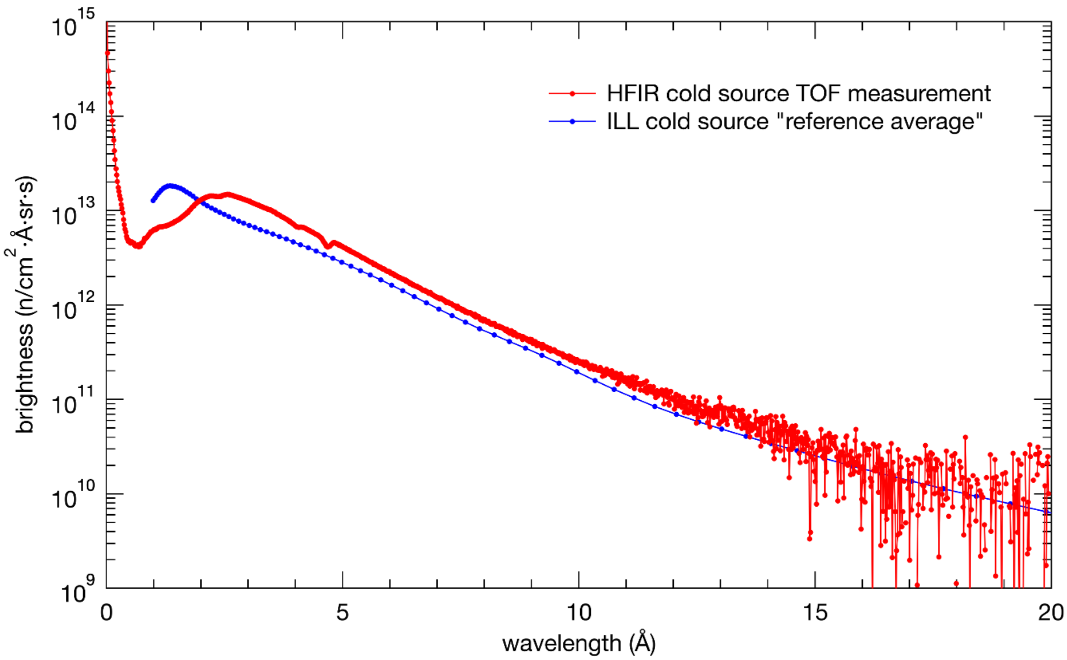



**Figure 7. (Red trace) time-of-flight spectrum of the cold source spectrum as measured, with all applicable corrections to the absolute scale.** Bragg edges from aluminum can be seen, for example around 5 Å. The blue trace indicates the Institute Laue Langevin reference average brightness for the HCS and VCS cold sources.

One further general remark concerns ballistic guides. Ballistic guides were considered for the HFIR guide hall, and it was decided to not pursue such a concept, with the exception of the IMAGING beamline. The overall conclusion was that ballistic guides would provide marginal benefit and would involve significant additional technical and engineering complications. The main underlying reasons are the limited divergence that can be pulled through the internal beam tube collimator and the strong horizontal curvature of the majority of the beams.

# 3. SCIENTIFIC REQUIREMENTS FOR INDIVIDUAL BEAMLINES

This section summarizes the scientific requirements for individual beamlines that fall within the scope of this review. These requirements include the optical transport of the neutron beams from the source to the instruments, and the respective footprint for each instrument on the guide hall floor. All beamlines have some requirements in common:

- The neutron guides are adequately separated to allow for efficient operation of each beamline and its commonly used scientific equipment.
- The neutron guides are adequately separated to allow for appropriate shielding.
- The design of the guides includes gaps for shutters, monitors, attenuators, and velocity selectors in appropriate (beamline-specific) locations.
- Each instrument has its own secondary shutter in the neutron guide hall.

## 3.1 NB-1 IMAGINE

IMAGINE is a macromolecular diffractometer that is designed to measure single crystal diffraction from samples with large unit cells (up to 150 Å on edge) in quasi-Laue mode. The instrument usually measures with a finite wavelength band of ~1.2–1.5 Å width. Depending on the size of the unit cell, it is necessary to change the lower and upper boundaries of the band independently to reduce the occurrence of overlapping Bragg peaks.

The following functional requirements have been set for the IMAGINE beamline at NB-1.

- The beam size at the sample shall be up to 2 mm horizontally and 2 mm vertically, i.e. up to 4 $mm^2$.
- The beam divergence at the sample shall be 0.2° FWHM horizontally and vertically.
- The lower boundary of the wavelength band incident on the sample can be set to 2.0, 2.8, or 3.3 Å.
- The upper boundary of the wavelength band incident on the sample can be set to 3.0, 3.3, 4.0 or 4.5 Å, or altogether removed (meaning the instrument receives the entire spectrum above the lower boundary of the wavelength band—Laue mode).
- The lower and upper boundaries of the wavelength band can be set independently.
- The footprint of the instrument enclosure shall be large enough to accommodate dynamic polarization equipment and other commonly used optical components, as well as future polarization and detector upgrades.
- The distance from the beam to any wall shall be at least 2 m.

## 3.2 NB-2 NEUTRON SPIN ECHO AND LARMOR

The neutron spin echo instrument at NB-2 will be a long-wavelength beamline that will use wavelengths of 8 Å and longer. Conceptually, it follows the generic IN11/IN15 type design with two long solenoids, one of which is in a fixed position on the incident side and the other moves around on a spectrometer arm.

A specific detail unique to this beamline is that the neutron guide exit is far away from the sample, at 3 to 4 m. The reason for this requirement is specific to the neutron spin echo technique. This instrument will establish two regions around the sample (before and after scattering) in which the neutron spins precess in highly homogeneous magnetic fields. No bounces in a guide can be tolerated in this region, as they would introduce path length differences than one cannot correct. The beam between the guide exit and the sample will be shaped by a series of apertures that trim the beam cross section successively down to the desired size at the sample.

Larmor will be a test beamline built at NB-2 before funding for the construction of the full spin echo beamline is obtained. This beam will be used to support the in-house development of neutron beam polarization devices.

The following functional requirements have been set for the spin echo beamline at NB-2.

- The beam size at the sample shall be 30 mm horizontally and vertically.

- The beam divergence at the sample shall be 0.8° half-width at half maximum (HWHM) horizontally and vertically.

- The optical transport from the source to the guide exit will be optimized for wavelengths of 8 Å (and longer).

- The instrument area will be large enough to allow the spectrometer arm to move to any scattering angle up to 120°.

### 3.3 NB-3 BIO-SANS

Bio-SANS at NB-3 is a conventional reactor SANS instrument that specializes in studying biological and soft matter materials.

The following functional requirements have been set for the Bio-SANS beamline at NB-3.

- The beam transport shall be optimized for 4 Å (and longer) neutrons but will allow the transmission of any wavelength down to 3 Å that can pass the velocity selector.

- The beam size at the guide exit shall be 40 mm horizontally and vertically.

- The beam divergence at the guide exit shall be 0.5° HWHM horizontally and vertically at 3 Å.

- The “natural” beam size at the sample shall be 40 mm horizontally and vertically but can be reduced with slits.

- The natural beam divergence at the sample shall be 0.5° HWHM horizontally and vertically at 3 Å but can be reduced to 0.15° HWHM horizontally and vertically with the collimation section between guide and sample.

- The sample area will be 2 m wide (1 m on each side of the sample, upstream and downstream) and will be in the area covered by an overhead crane.

- The sample area will be accessible from above and from one side.

## 3.4 NB-4 IMAGING

IMAGING at NB-4 is a flexible cold neutron imaging station with many applications that reach into the thermal part of the available spectrum.

The following functional requirements have been set for the IMAGING beamline at NB-4.

- The collimation (*L/D* ratio) shall be tunable between 150 and 2000.
- With an *L/D* ratio of 150 (high flux, low spatial resolution), the polychromatic flux on the sample shall exceed $10^9$ n/cm$^2$/s.
- The longest pin-hole to sample distance shall be *L*=15 m.
- If a guide system is inevitable, it must be designed in such a way that it minimizes beam artifacts and divergence inhomogeneities across a broad range of neutron wavelengths. If a beam diffuser is required, it shall be positioned upstream of the beamline aperture selector. The beam delivery system must also allow a future upgrade with a ballistic guide feeding a system of Wolter mirrors.
- The field-of-view (FOV) shall be defined as a (rectangular) area on the detector in which the beam intensity does not drop below 75% of the maximum.
- The FOV and beam divergence at the sample shall be tunable between a FOV of 10×10 cm (for the longest *L*-value), allowing a spatial resolution of 50 μm on the detector and a FOV of 5×5 mm with a spatial resolution of 5 μm.
- The floor space around the sample position needs to be sufficient to allow the complex and varied experimental settings typical for an imaging beamline. These include polarized imaging, multimodal imaging (neutrons in combination with fluorescence, infrared, or x-ray equipment). The floor should be well leveled.
- The perimeter of the beamline needs to be well shielded, which requires additional space.

## 3.5 NB-5 GP-SANS

GP-SANS at NB-5 is a conventional reactor general-purpose SANS instrument.

The following functional requirements have been set for the GP-SANS beamline at NB-5.

- The beam transport shall be optimized for 4 Å (and longer) neutrons but will allow the transmission of any wavelength down to 3 Å that can pass the velocity selector.
- The beam size at the guide exit shall be 40 mm horizontally and vertically.
- The beam divergence at the guide exit shall be 0.5° HWHM horizontally and vertically at 3 Å.
- The natural beam size at the sample shall be 40 mm horizontally and vertically but can be reduced with slits.

- The natural beam divergence at the sample shall be 0.5° HWHM horizontally and vertically at 3 Å but can be reduced to 0.15° HWHM horizontally and vertically with the collimation section between guide and sample.

- The sample area will be 2 m wide (1 m on each side of the sample, upstream and downstream) and will be in the area covered by an overhead crane.

- The sample area will be accessible from above and from one side.

### 3.6 NB-6 MANTA

MANTA at NB-6 will be a cold triple-axis spectrometer. Initially it will use the existing C-TAX back end, but an upgrade with a multiplexed back end is being planned.

The following functional requirements have been set for the MANTA beamline at NB-6.

- The smallest FWHM of the beam size on the sample shall be 20 mm horizontally and vertically.

- The maximal beam divergence at the sample shall be 2.0° HWHM horizontally and 3.0° HWHM vertically.

- The beamline is optimized to operate with an incident wavelength (energy) between 1.8 Å (25 meV) and 5.7 Å (2.5 meV). Longer-wavelength neutrons will be available, but the instrument will not be optimized to use them.

- The horizontal radius of curvature of the monochromator shall be adjustable, depending on the incident wavelength.

- The beamline can operate with a 15 T (vertical field, uncompensated) cryomagnet at the sample position.

## 4. PROPOSED NEW GUIDE SYSTEM

The design of the guide system presented in this section is considered "final" in the front-end part up to the boundary between the transition building and the guide hall building. The conceptual designs for the individual beamlines downstream of that point are still in progress.

### 4.1 COMMON FRONT-END SECTIONS

The HB-4 beam tube and the cross-section of the integrated collimator are shown in Figure 2. The beam tube is followed by a rotary shutter and then the entrance to the guide system. The shutter consists of a rotating drum with a vertical rotation axis with penetration for three neutron beams when in the open position.

The McStas calculation shows (Figure 8) that the beam profile coming out of the beam tube collimator is not ideally homogeneous because the internal piping (for example, hydrogen load lines feeding the cold source) creates shadows. Further, the beam coming out of the collimator is not centered with respect to the source but is vertically offset because the collimator itself is not a symmetric piece. Individual neutron beams toward instruments should view the center of the source, but the offset has the consequence that most beams are pointing upward.

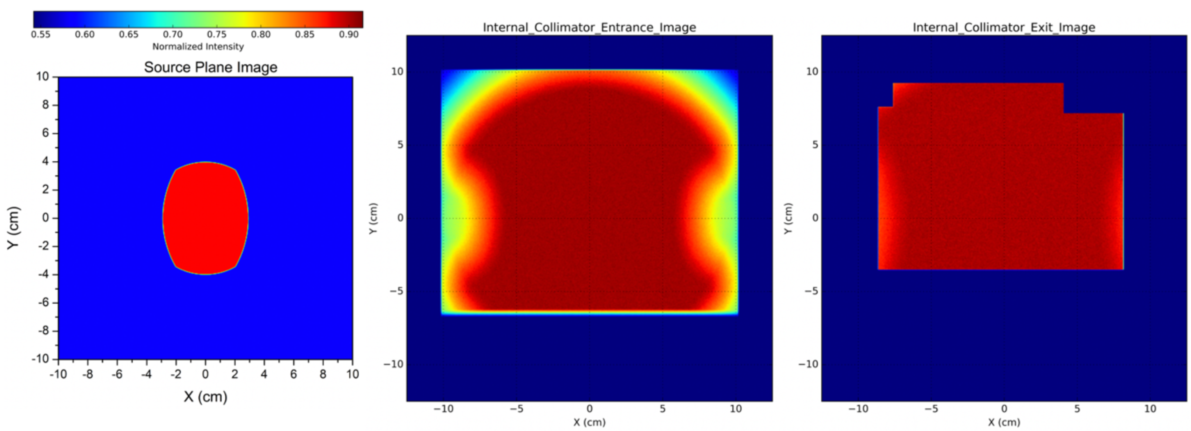



**Figure 8. Calculated McStas histograms of the beam profile coming off the source (left) and going in and coming out of the collimator (center and right), looking upstream into the cold source.** The three histograms are on a common centerline vertically. Inhomogeneities in the beam profile (left and right) are on the 10% level and are due to shadows from the piping upstream of and internal to the collimator.

The definition of the individual beams at the shutter entrance and exit is shown in Figure 9 and Figure 10. Ultimately, the viewable solid angle from the cold source is subdivided into six beams; but at the shutter position, it is divided into just three channels. The reason is that when the cold source is viewed through the shutter, the beams can already be separated horizontally but still nominally overlap in the vertical plane. By the time the guide system begins, all six beams are spatially separated. The guides begin at 4.64 m from the viewable surface of the cold source (that is, downstream of the shutter) so the guides will be under-illuminated for neutron wavelengths greater than about 4 Å, depending on the exact height and width of each guide entrance.

It is possible to place neutron guides in the shutter, to bring them closer to the source by about 0.5 m, but not in the HB-4 beam tube. For the sake of completeness, the implications of reflecting surfaces in the

HB-4 beam tube collimator were studied; and it was concluded that it was not desirable to place any neutron guide in this location.

The option to place neutron guides in the shutter was evaluated for each beamline individually and carefully, because it has major engineering implications for the shutter design in terms of the accuracy and repeatability of the nominal "open" position (at present, there is no guide in the HB-4 shutter). The conclusion was that MANTA at the shutter-3 (SH-3) penetration clearly needs an *m*=3 guide coating in the shutter. The other beamlines are well served with an *m*=1 guide coating in the shutter insert and no vertical separation of the beams.

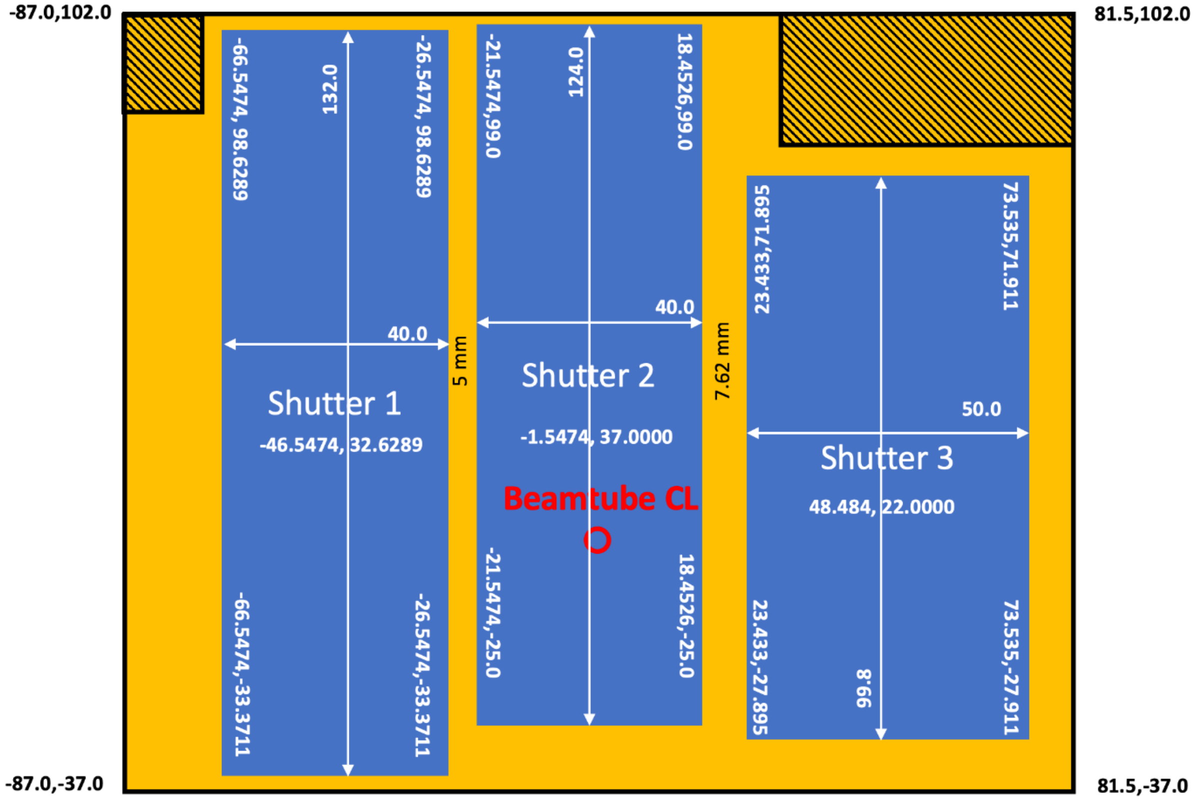



**Figure 9. The arrangement of the beams at the entrance of the primary HB-4 shutter, looking upstream into the cold source.** This is at a distance of 4.04 m from the source. The beams are split horizontally but not vertically. The red dot designates the horizontal beam tube center line.

Beamlines NB-1 (IMAGINE), NB-3 (Bio-SANS), and NB-4 (IMAGING) occupy the shutter penetration SH-1 (see Figure 11), with NB-3 matching the 0.5° incline of the current Bio-SANS beamline. IMAGING and Bio-SANS use SH-1 because SH-1 already makes a horizontal angle of 0.66° to the west of the HB-4 beam tube centerline. All three of these guides (NB-1, 3, and 4) will eventually (further downstream) curve to the west by more than 0.66°, so by using SH-1 these guides require less curvature. NB-5 (GP-SANS) and NB-2 (spin-echo, sample alignment) will occupy the SH-2 shutter penetration. The NB-5 guide has the same position and direction as the current GP-SANS guide, so the GP-SANS detector vessel can sit in the existing floor trench. NB-2 will be located at SH-2 rather than at SH-1 because the spin echo instrument can use a taller beam, and it will use longer-wavelength neutrons, so minimizing the guide curvature is less important. Note that this choice means that NB-2 will cross over NB-4 and NB-5. As mentioned previously, the NB-6 guide (MANTA) is on the east side of the beam and occupies the entire cross-section of the SH-3 shutter penetration.

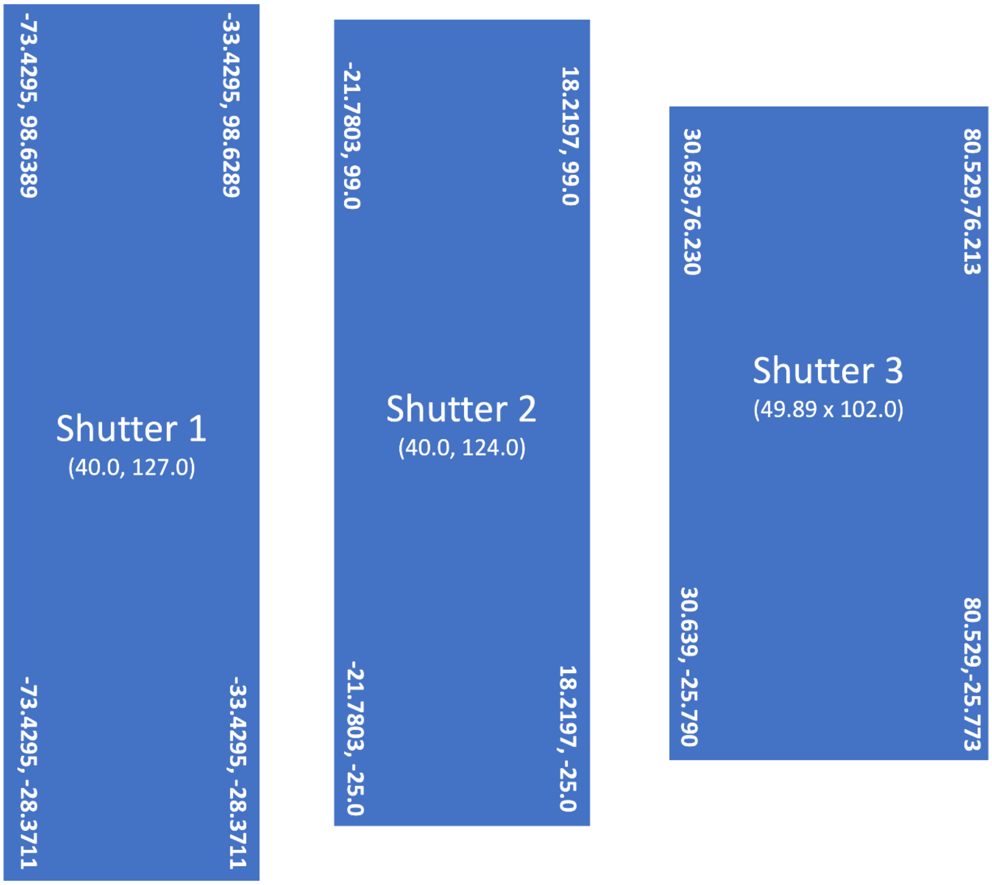



**Figure 10. The arrangement of the beams at the exit of the primary HB-4 shutter, looking upstream into the cold source.** This is at a distance of 4.64 m from the source. The beams are generally larger than at the entrance.

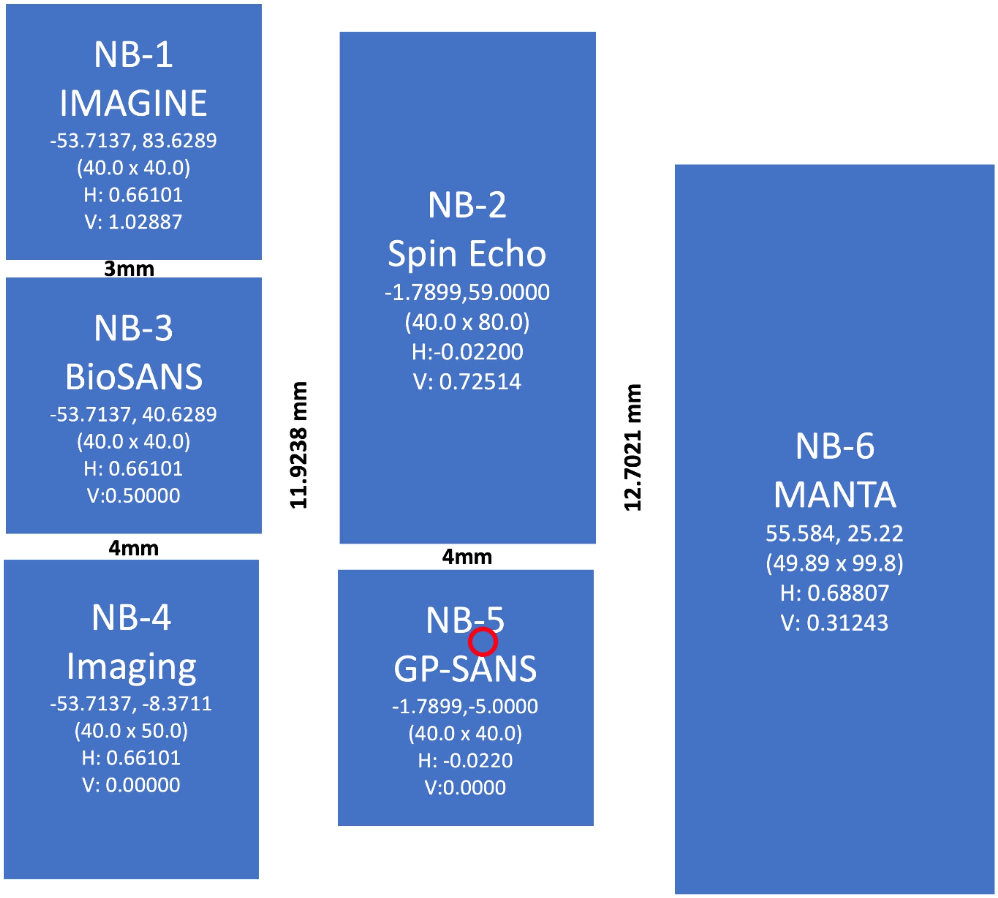



**Figure 11. The arrangement of the beams at the entrance to the guide system, looking upstream into the cold source.** The red dot designates the beam tube center line.

### 4.2 NB-1 IMAGINE

Beamline NB-1, which supplies neutrons to the IMAGINE macromolecular diffractometer has the greatest curvature of 12.7°. It uses a pair of band pass mirrors to select the wavelength band and an ellipsoidal mirror or nested Kirkpatrick-Baez mirror to image the entrance slit onto the sample position with a magnification of 0.3. This diffractometer operates in quasi-Laue mode with a wavelength band of 2.8 to 4.5 Å (or longer). The vertical and horizontal divergence on the sample should be 0.2° FWHM. At first glance, it would seem inappropriate for a guide that needs to transport 2.8 Å neutrons to have such a strong curvature. Fortunately, NB-1 does not need to transport more divergence than the imaging mirror can accept. The horizontal divergence accepted is on the order of 0.1°. Either a curved guide or a multi-segment optical filter can efficiently deliver the needed divergence.

The beam delivery system was split into two parts, guide and ellipsoidal mirror, which were considered separately. To optimize the neutron transport to the guide exit, regions of interest (ROIs) were defined along the beamline where *m*-values of the guide coating were held constant; but between regions, the coating was varied (Figures 12–16).

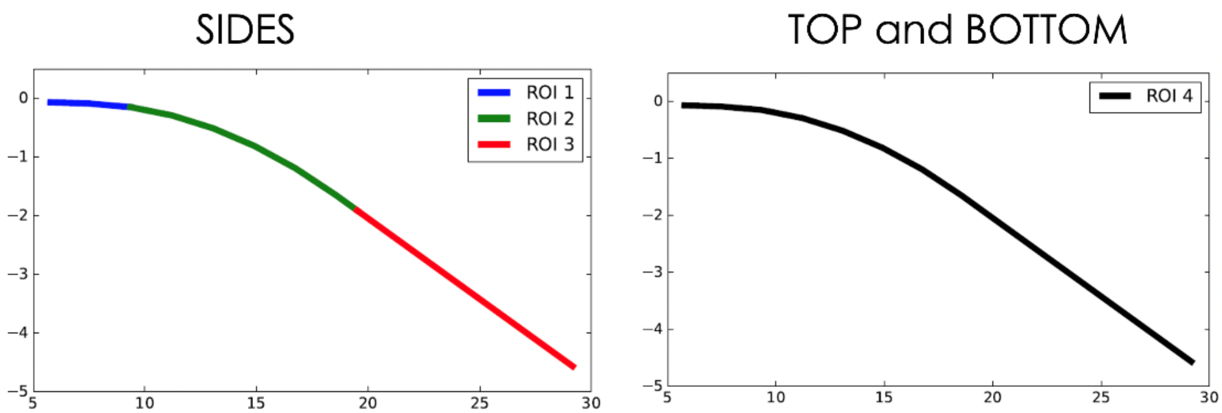



**Figure 12. Regions of interest for guide m-values at NB-1.** The units on the axes are meters. ROI-1 and ROI-3 are straight sections; ROI-2 is curved.

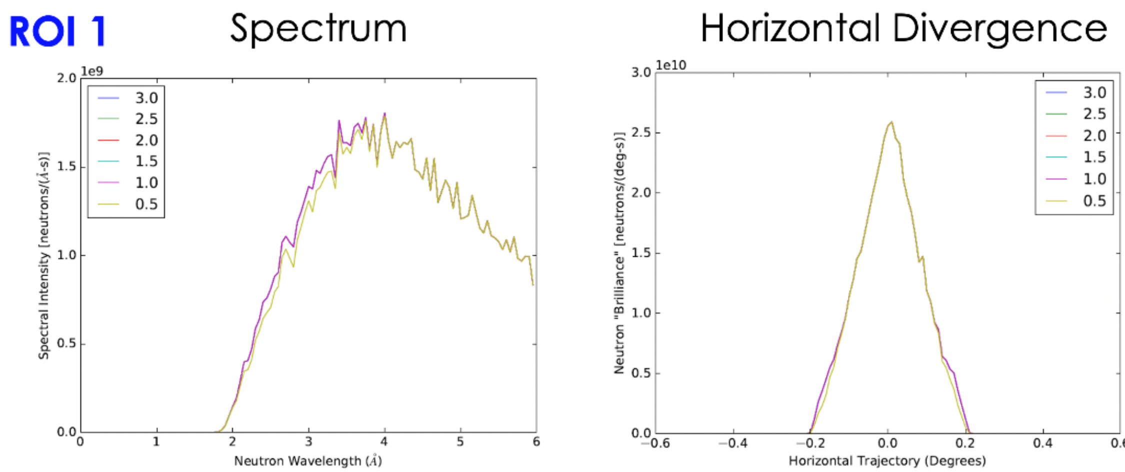



**Figure 13. Study of the effect of m-values in ROI-1.**

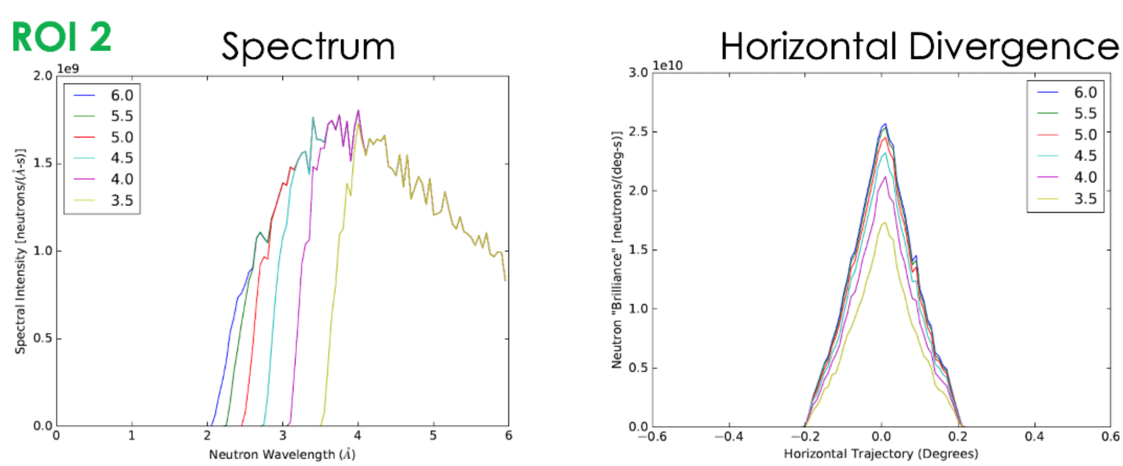



**Figure 14. Study of the effect of m-values in ROI-2.**

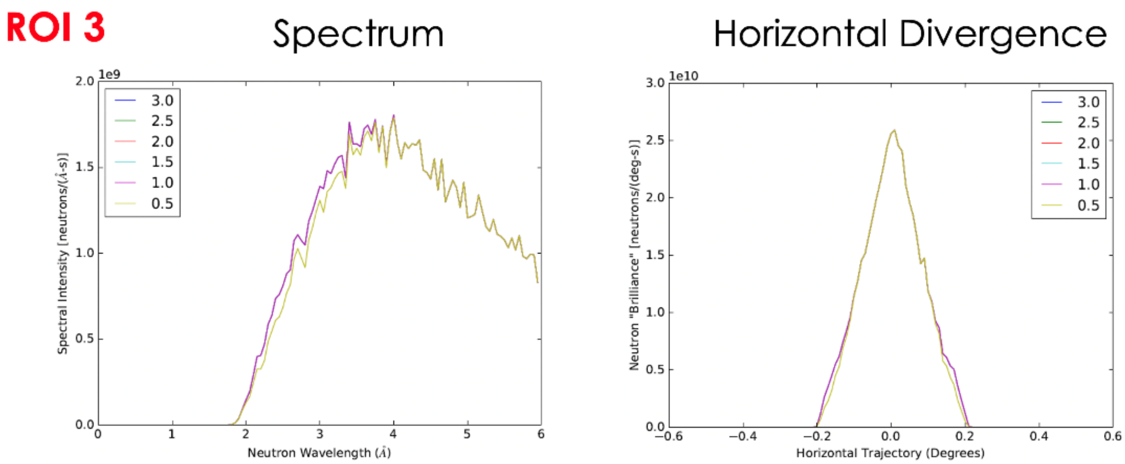



**Figure 15. Study of the effect of m-values in ROI-3.**

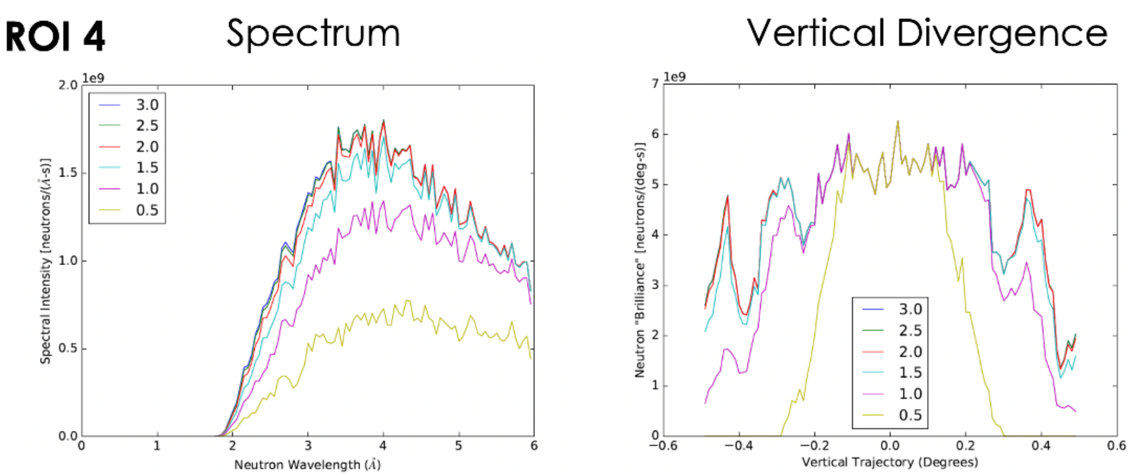



**Figure 16. Study of the effect of m-values in ROI-4.**

Final decisions on the choice of the *m*-values have not been reached at this point. With the exception of the curved section (ROI-2), the choice can be limited to *m*-values <~2.

The resulting intensity and divergence profiles at the guide exit are shown in Figure 17.

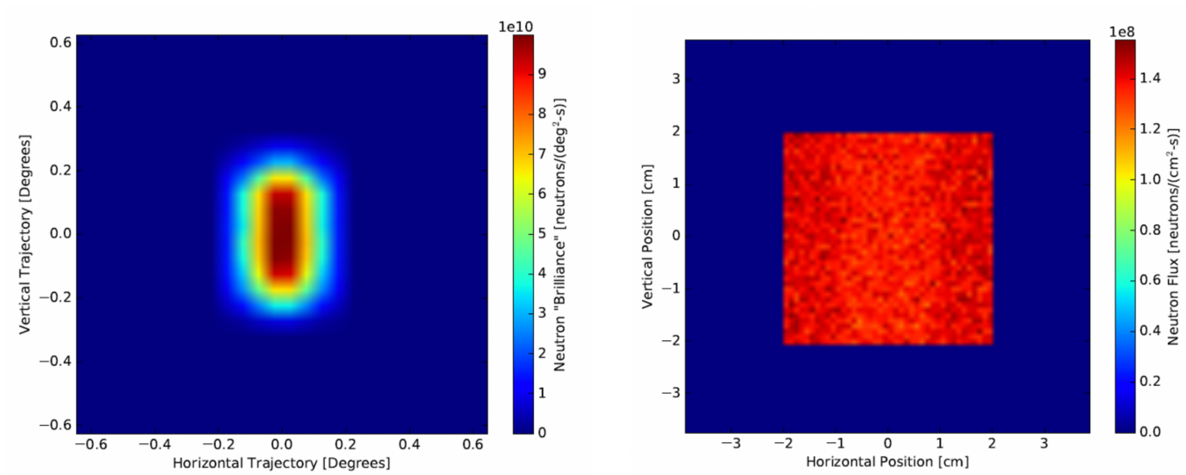



**Figure 17. Intensity and divergence profiles at the NB-1 guide exit.**

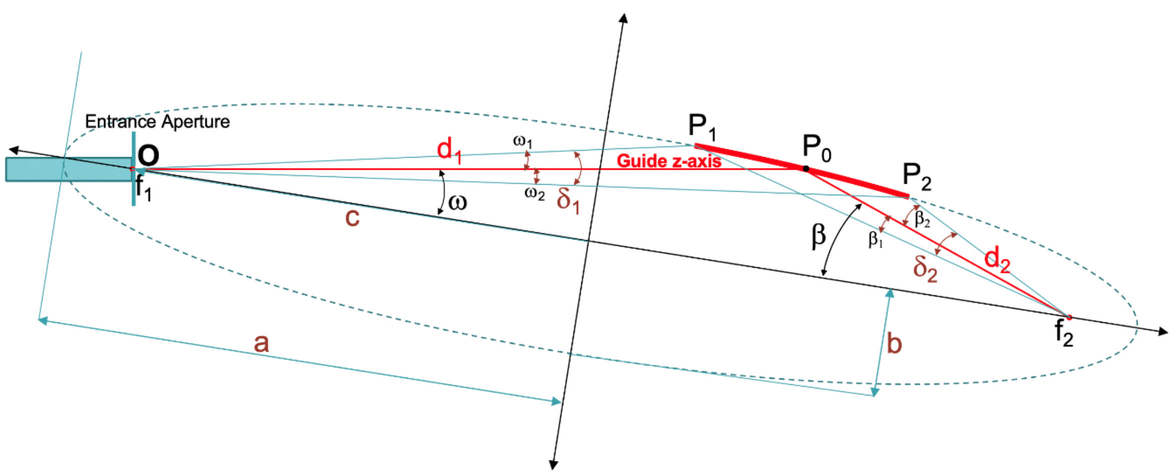



**Figure 18. Concept for an ellipsoidal mirror for IMAGINE.**

The existing IMAGINE beamline uses an ellipsoidal mirror to transport a spot-like beam on the sample. The same concept will be pursued for the future upgrade. This mirror will have a demagnification factor of ~3 and illuminate the sample with a beam size of up to 2×2 mm with a divergence of up to 0.4°×0.4° (full width). Final figures for brilliance transfer and flux on sample will be available when the mirror design is complete. As is the case for GP-SANS, the expectation is that a modest performance gain will be achieved, because the beamline design is fundamentally unchanged; the most important change will be the reduced distance (from ~5 to ~4 m) of the guide entrance to the source.

### 4.3 NB-2 NEUTRON SPIN ECHO AND LARMOR

The spin echo instrument and the Larmor test beam will use mostly long-wavelength neutrons, 8 Å and longer. Therefore, the NB-2 guide can be positioned west of the Bio-SANS detector vessel with little loss in performance (Figure 19). Beamline NB-2 will employ a double logarithmic spiral to route the beamline west of the Bio-SANS detector vessel and into the south-end extension of the guide hall.

The spin echo instrument is new and is not yet funded; so when the reactor resumes operation following the beryllium reflector replacement, a Larmor methods development instrument will occupy the temporary end guide position on NB-2. The sample alignment station, NB-2A, will employ a fixed monochromator in the NB-2 guide, about 10 m beyond the Bio-SANS velocity selector, and will be a side instrument.

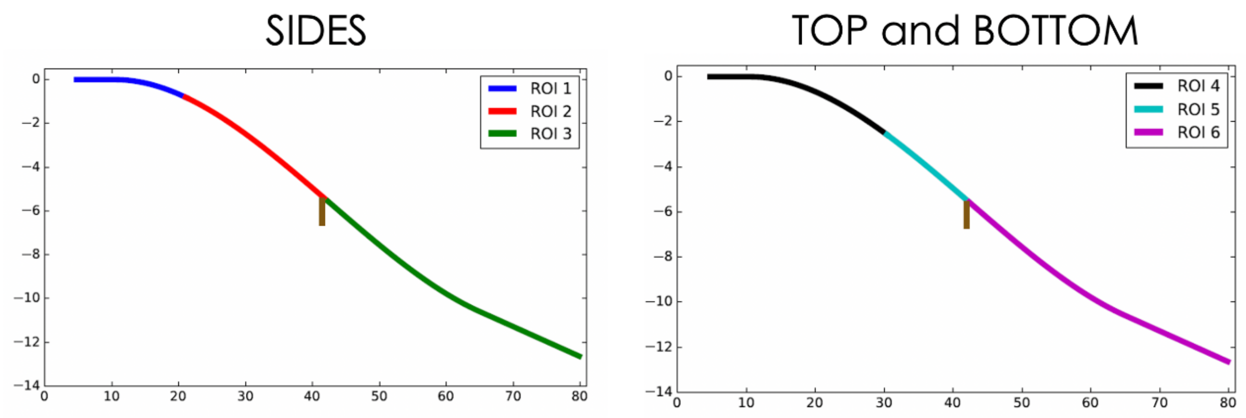



**Figure 19. Beamline layout of the neutron spin echo beamline at NB-2 in McStas.** The ROIs mark regions with constant guide coating. ROI-1 to 3 are relevant for the side coating, ROI-4 to 6 for top and bottom coating.

The beam size of the spin echo guide was set by the requirement that the guide exit should be about 4 m upstream of the sample position, which is an unusually long distance. This comes from the fact that the neutron trajectories have to be exactly straight in the regions where the neutron spins precess, which is several meters upstream and downstream of the sample. To illuminate the sample with a meaningful divergence, a guide cross section of 8×4 $cm^2$ was chosen for the spin echo beamline. The beam cross section will simply be tapered down with apertures between the guide exit and the sample position.

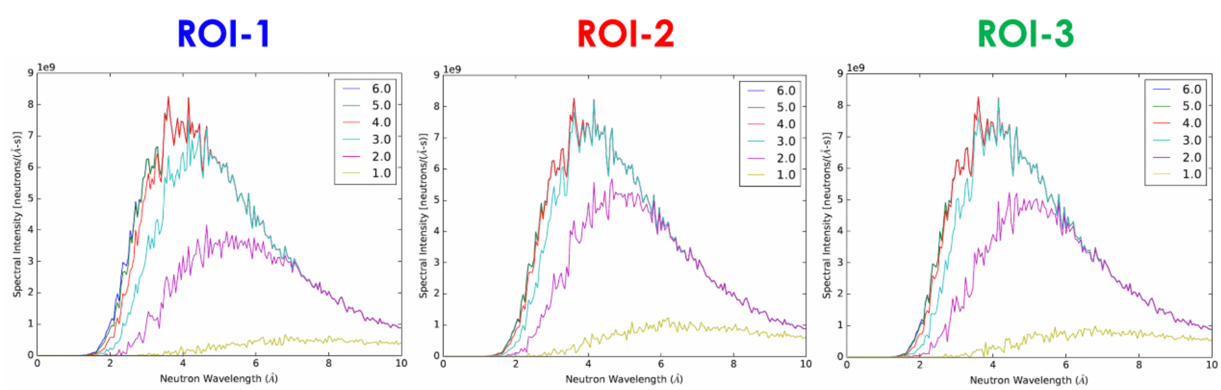



**Figure 20. Optimized side coating for the spin echo beamline.** ROI-1 refers to upstream of the 20 m position and ROI-2 is downstream of the 40 m position. In the front (ROI-1 and 2) rather high m-values will be needed, but in ROI-3, m=2 is sufficient.

When the curvature of the beamline was set as described above, the *m*-values of the guide coating were optimized in a last step of the design (Figure 20 and Figure 21). The results are slightly different for the side (left/right) and upper/lower (top/bottom) coatings. The single crystal alignment station will use significantly shorter-wavelength neutrons, ~2.5 Å, and the requirement to transport these neutrons through ROI-2 sets the *m*-values for the side guide coating.

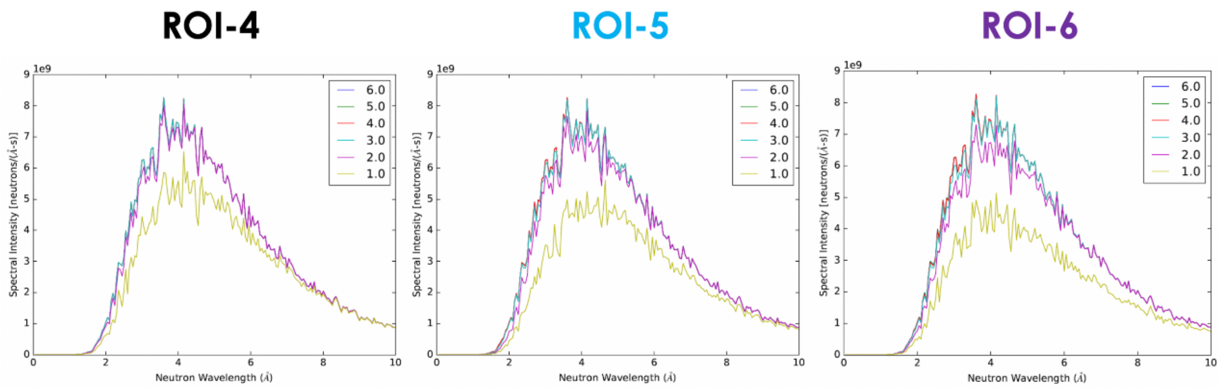



**Figure 21. Optimized top/bottom coating for the spin echo beamline.** ROI-3 refers to upstream of the 30 m position, ROI-5 is downstream of the 40 m position, and ROI-4 is in between. It is sufficient to have m=2 in ROI-4 to 6.

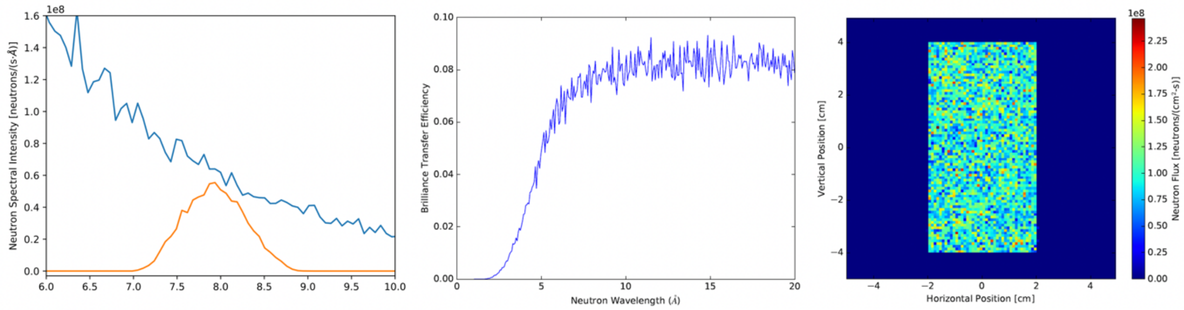



**Figure 22. Resulting spectrum at neutron spin echo after all optimizations (left), brilliance transfer to the sample at 4 m from the guide exit, middle) and guide exit beam image (right).**

The total simulated intensity at the sample position between 7 Å and 9 Å is $4.8 \times 10^7$ n/s with a velocity selector at 8 Å and 11% FWHM. The spectrum is shown in Figure 22. The divergence at the sample follows from the 'natural' illumination from the guide exit, 0.9°. full width horizontally and 1.5° full width vertically.

### 4.4 NB-3 BIO-SANS

The current implementation of NB-3 (Bio-SANS) uses an optical filter followed by a straight guide. In the new instrument landscape, space must be provided between the two SANS instruments for the IMAGING beam at NB-4. To make room for IMAGING at NB-4, the Bio-SANS detector tank will be moved sideways from its current location by about half its width. Thus, the beamline will be more strongly curved than it is currently. In the new configuration, a conventional curved guide (Figure 23) will clearly outperform an optical filter for Bio-SANS, as was confirmed by simulation. To minimize the losses, the amount of curvature was also minimized.

Currently the beamline is inclined upward by 0.5° because (as discussed earlier) the Bio-SANS beam already in the beam tube is looking down onto the center of the cold source. The decision was made to keep the incline, because doing so will make installing the tank in its new location easier; moreover, there would be an additional loss in flux at the sample position if the beam were bent back horizontally.

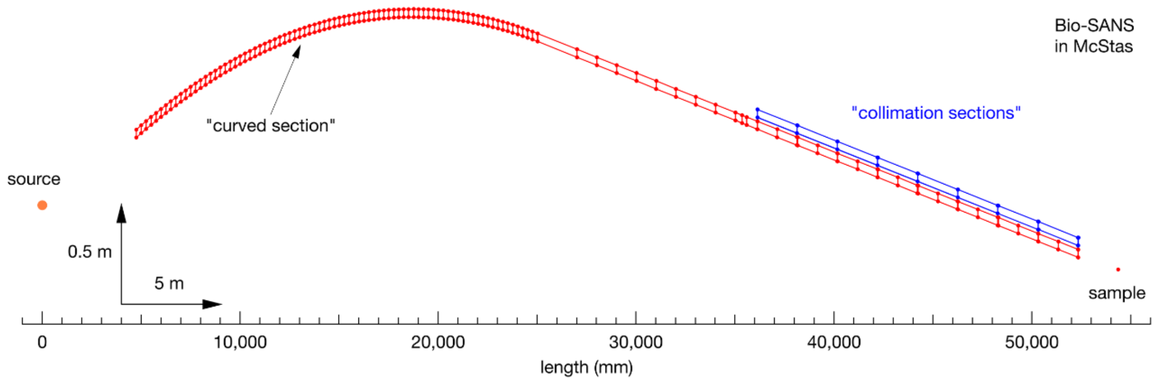



**Figure 23. Bio-SANS model in McStas.** The radius of curvature in the curved section is constant along the length. It appears to be different in the figure only because the vertical scale is stretched.

Changing the instrument resolution for a SANS effectively means changing the beam divergence on sample, and the sample to detector distance, to resolve a minimum scattering angle as needed for a particular science application. The traditional method of doing so at HFIR is as follows. The permanently installed neutron guide ends at ~18 m upstream of the sample position. Between the guide exit and the sample position are eight individual guide sections, each 2 m long, which can be independently translated horizontally in and out of the beam and exchanged with simple flight tubes. These are referred to as "collimation sections." The more of these guide sections that are "active" in the beam, the higher the divergence transported to the sample.

The curvature of the beam results in a strongly structured horizontal divergence profile at the guide exit, to a degree that raises concerns regarding negative implications for the sample illumination and ultimately regarding the scientific value of the data obtained. Various possibilities have been considered for mitigating this transport problem by design. The following four configurations will be compared:

- Single Channel: The guide has a simple rectangular cross section all along the curved and straight sections. The overall cross section is constant, 40×40 mm$^2$, along the entire beamline.
- 3-channel: The curved section has three evenly spaced channels ("slits" in McStas) and is followed by a straight section with rectangular (single-channel) cross section. The overall cross section is constant, 40×40 mm$^2$, along the entire beamline.
- Squeezer: The curved section is not split in channels but gradually narrows to a 20 mm width at the end. The downstream straight section, again rectangular, starts at a 20 mm width and gradually expands to 40 mm at the guide exit.
- Octo: The curved section is the same as in the squeezer configuration, and the following straight section gradually converts the cross section to octagonal. The collimation sections also feature guides with octagonal cross section.

The configurations considered are illustrated in Figure 24. The rationale for the 3-channel configuration is that additional reflecting surfaces will increase the number of zig-zag reflections at the expense of garland reflections. Without channels, it is observed that about 80% of the neutrons exiting the curved section would be in the outside half of the exit window. It was found that increasing the numbers of channels beyond three had no significant overall positive effect. The rationale for the squeezer configuration is the same—increasing the beam divergence and the number of reflections in the curved section. The degree to which the beam is squeezed can be freely chosen, and 20 mm (factor 2) was found to be a reasonable choice. Finally, the rationale for the octagonal guide was that this shape introduces a mixing of the horizontal and vertical divergence (which is not affected by the horizontal curvature), effectively scrambling the phase space more quickly along the length of the beamline (Figure 25).

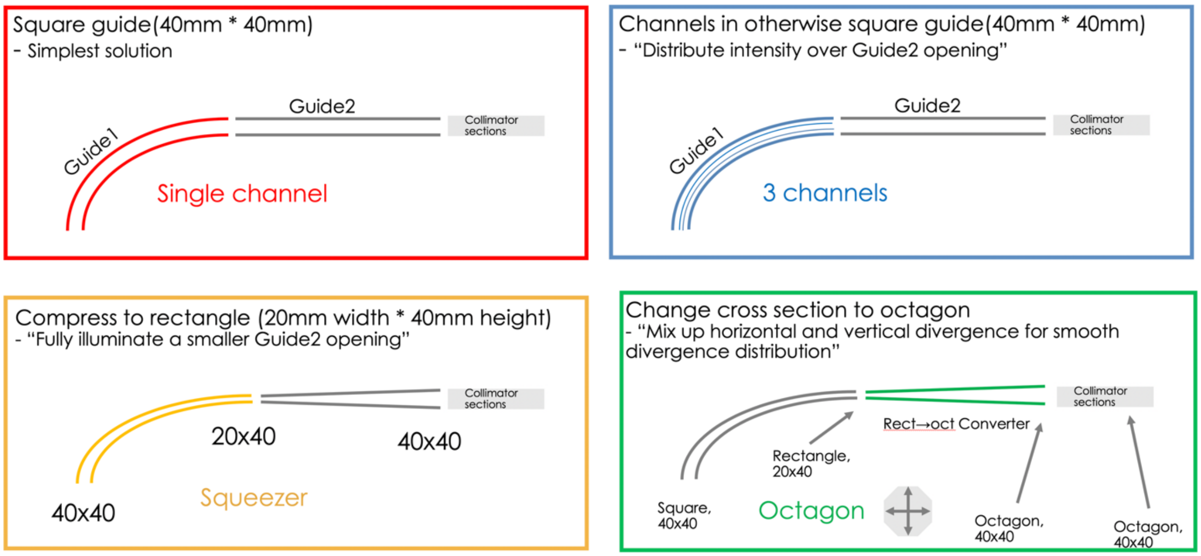



**Figure 24. Four representative configurations considered for the Bio-SANS optical beamline design.**

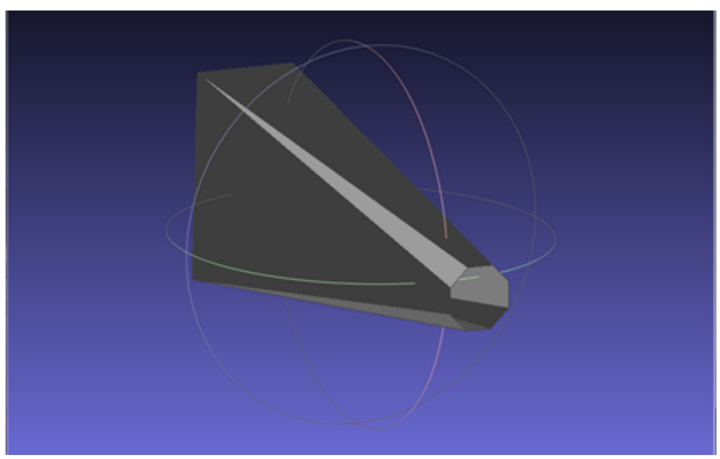


**Figure 25. A 3D rendering of the rectangular-to-octagonal cross section converter piece.**

For this case, a McStas simulation of the beam profile incident on the sample is insufficient to judge the quality of a design. It was decided to include the sample scattering in the simulation and to compare simulated detector patterns. To this end, two different samples were simulated, which represent typical scattering laws encountered at Bio-SANS:

- 4-m, high intensity: an isotropic scatterer with a *d*-spacing of 58 Å, with a sample-to-detector distance of 2.25 m and 7 collimation sections, meaning 4 m of collimation length (Figure 26)
- 10-m, high resolution: an isotropic scatterer with a *d*-spacing of 120 Å, with a sample-to-detector distance of 7 m and 4 collimation sections, meaning 10 m of collimation length (Figure 27)

The wavelength was set to 6 Å in both cases with a velocity selector. In all cases, the beam at the sample position was defined by a 2 cm diameter circular aperture.

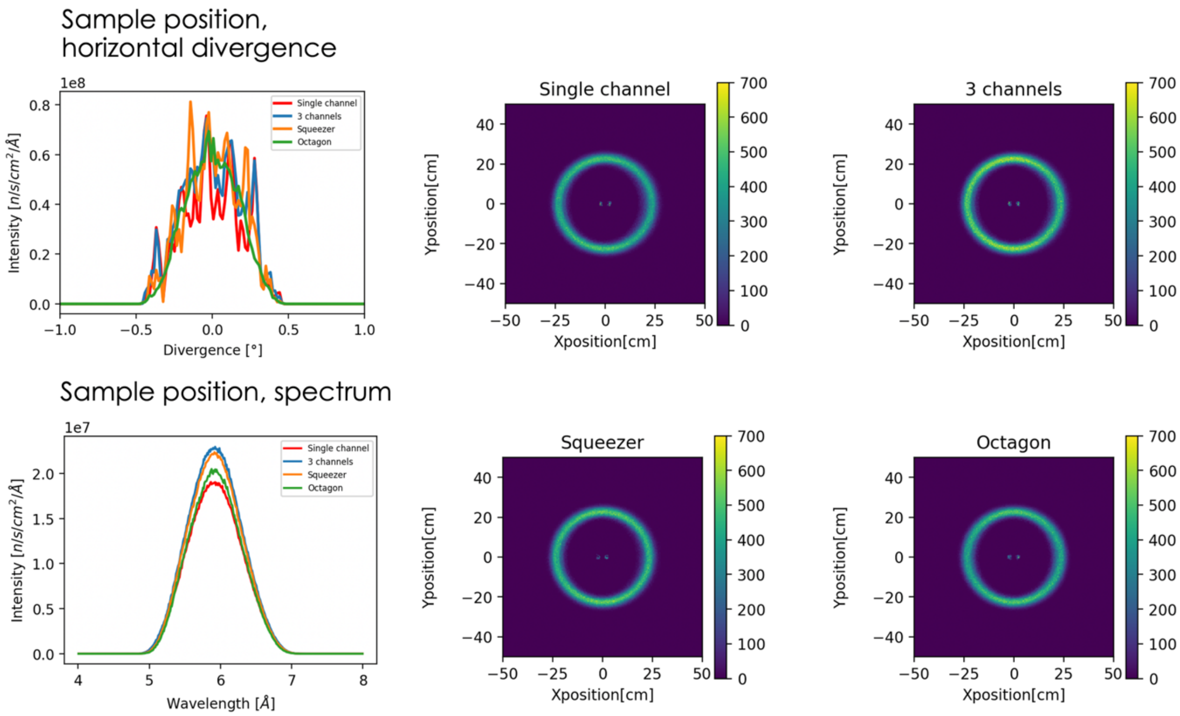



**Figure 26. High-intensity study with details as presented for the 4 m configuration.** Horizontal divergence at the sample position (top left), spectrum at the sample position (bottom left), red trace (top center scattering pattern): single channel, blue trace (top right scattering pattern): 3-channel; orange trace (bottom center scattering pattern): squeezer; green trace (bottom right scattering pattern): octo.

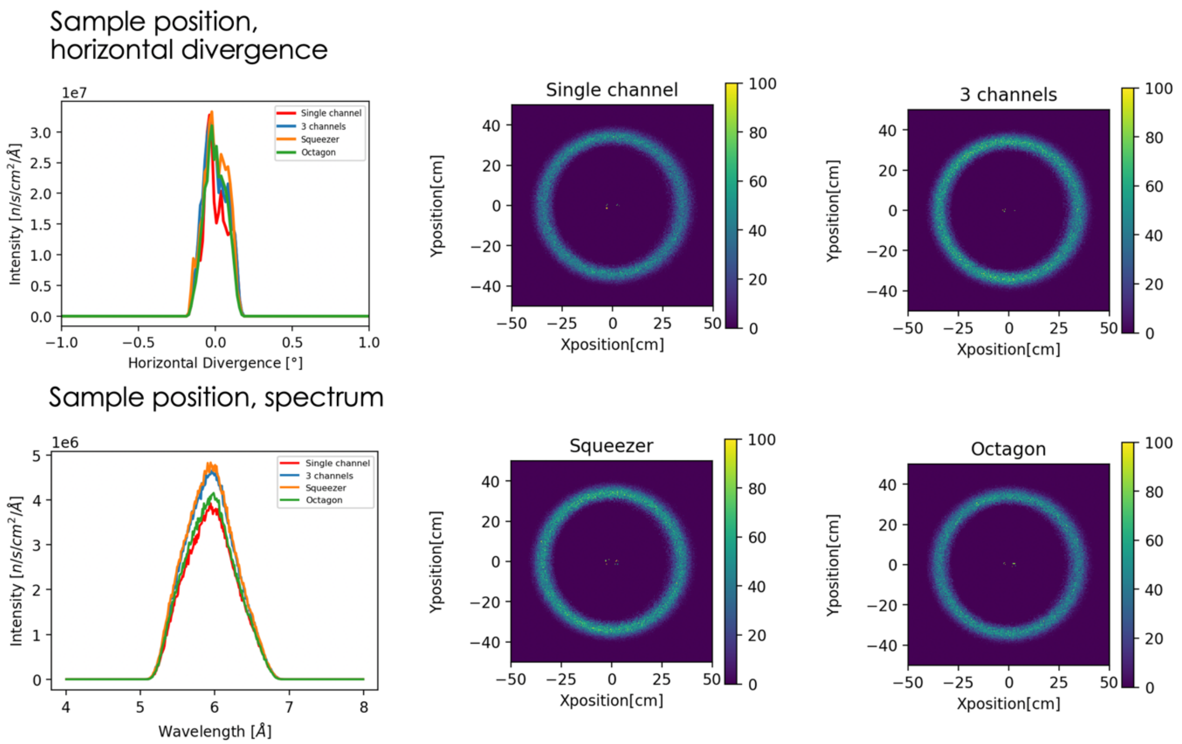



**Figure 27. High-resolution study with details as presented for the10 m configuration.** Horizontal divergence at the sample position (top left), spectrum at the sample position (bottom left), red trace (top center scattering pattern): single channel, blue trace (top right scattering pattern): 3-channel; orange trace (bottom center scattering pattern): squeezer; green trace (bottom right scattering pattern): octo.

These simulations demonstrate that the horizontal divergence pattern appears to be much improved with the octagonal guide design, in particular for the high-intensity case. However, the sample scattering seems to be acceptable in either case.

Simulations of the sample illumination are shown in Figures 28 and 29. All designs pass the basic requirement of a homogeneous sample illumination. A quantitative analysis shows that in all cases, histograms of the intensity across the sample and the divergence distribution across the sample are within 10% between the right half and left half.

The overall conclusion from these studies is that the conceptual design will be the squeezer configuration, but it may need further refinement.

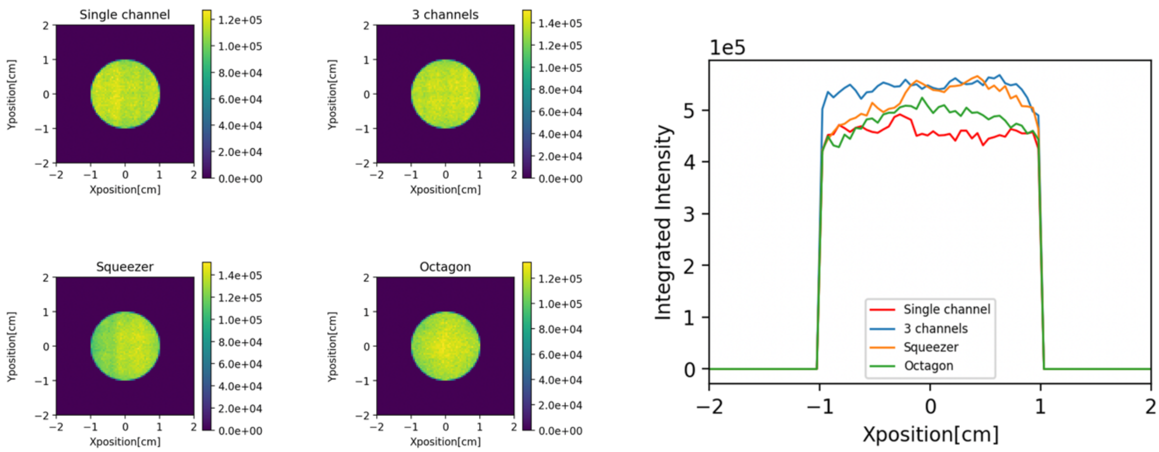



**Figure 28. Simulation of the sample illumination and the homogeneity of the beam across the sample position for the high intensity case.** Top left: single-channel (red trace), top center: 3-channel (blue trace), bottom left: squeezer (orange trace), bottom center: octo (green trace). A horizontal cut through the centerline is shown on the right-hand side.

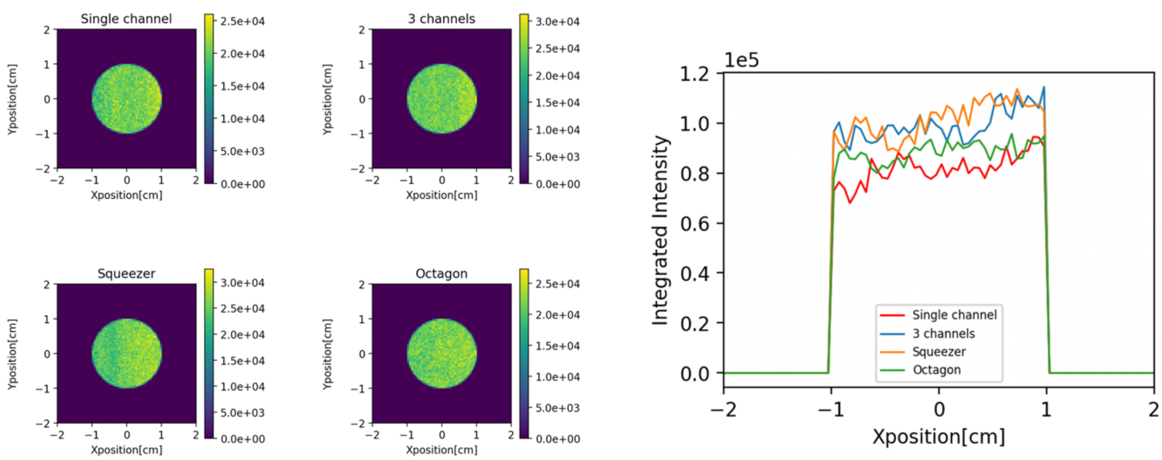



**Figure 29. Simulation of the sample illumination and the homogeneity of the beam across the sample position for the high resolution case.** Top left: single-channel (red trace), top center: 3-channel (blue trace), bottom left: squeezer (orange trace), bottom center: octo (green trace). A horizontal cut through the centerline is shown on the right-hand side.

The analysis of the *m*-values of the guide coating is preliminary at this time. To transport a 4 Å center wavelength to the sample position, guide coatings with m~4 are required, mostly along the length of the beamline (Figure 30).


**Figure 30. Study of the m-values in the Bio-SANS guide needed to transport a center wavelength of λ=4 Å (top row) and λ=5 Å (bottom row).**

In the wavelength range in which Bio-SANS operates, at λ~6 Å and longer, it stands to gain ~50% flux on sample in a like-to-like comparison between the existing instrument and the new design. However, the most important gain for this instrument is that it will be able to access shorter-wavelength neutrons below the present cutoff, down to λ~4 Å.

### 4.5 NB-4 IMAGING

As is explained earlier, the best solution for the IMAGING beamline, other than remaining in its current place (which would be impossible, because the C-TAX instrument will be installed in that location), is to route the beam between the two SANS tanks. Any other location for the IMAGING beam would require bending the beam to an extent that would severely compromise the transport of ~2 Å neutrons to the sample position. Since there currently is no dedicated thermal IMAGING instrument at ORNL, IMAGING at NB-4 places a strong emphasis on this wavelength range.

The NB-4 guide will need to be curved to fit within the available space. The parameters of the curve were optimized to give the best short-wavelength transport. A polynomial approximation was used during the optimization to speed up the process. The optimization also included a straight guide section at the end. Ultimately, the optimization process drove the shape of the curve to a configuration that could be closely approximated by a simple curved guide with circular curvature; so that configuration is being used rather than the more complicated formal logarithmic spiral.

Much as is the case for the Bio-SANS beamline at NB-3, a significant structure is obtained in the horizontal divergence distribution. The NB-4 beam is less curved than the NB-3 beam, but the sensitivity to this structure increases when it is imaged directly via a pinhole (as no scattering will smear out the divergence profile.

Again, a comparative study was conducted with traditional rectangular and unconventional octagonal guides (Figure 31). The rationale for the octagonal guide was described previously. The curved guide section gradually narrows down for the same reason as at Bio-SANS: to mitigate the observed uneven distribution of neutrons exiting the curved section with a strong tendency towards the outside of the curve. Final parameters for the cross-section reduction and *m*-values in the guide are left to be optimized. A velocity selector can be remotely positioned when needed for imaging. The aperture system, flight tubes, sample table and detectors are positioned downstream of the velocity selector. A variable distance of 8 to 13 m between the aperture system and the beam stop is also illustrated in Figure 31.Three *L/D* settings were simulated, with the final (circular) pinhole 59 cm downstream of the guide exit (to leave space for a velocity selector) and the detector at *L*=8.7 m from the pinhole. The settings were high *D*=0.005 m (*L/D*=1,740), medium *D*=0.01 m (*L/D*=870), and low *D*=0.038 m (*L/D*=230).

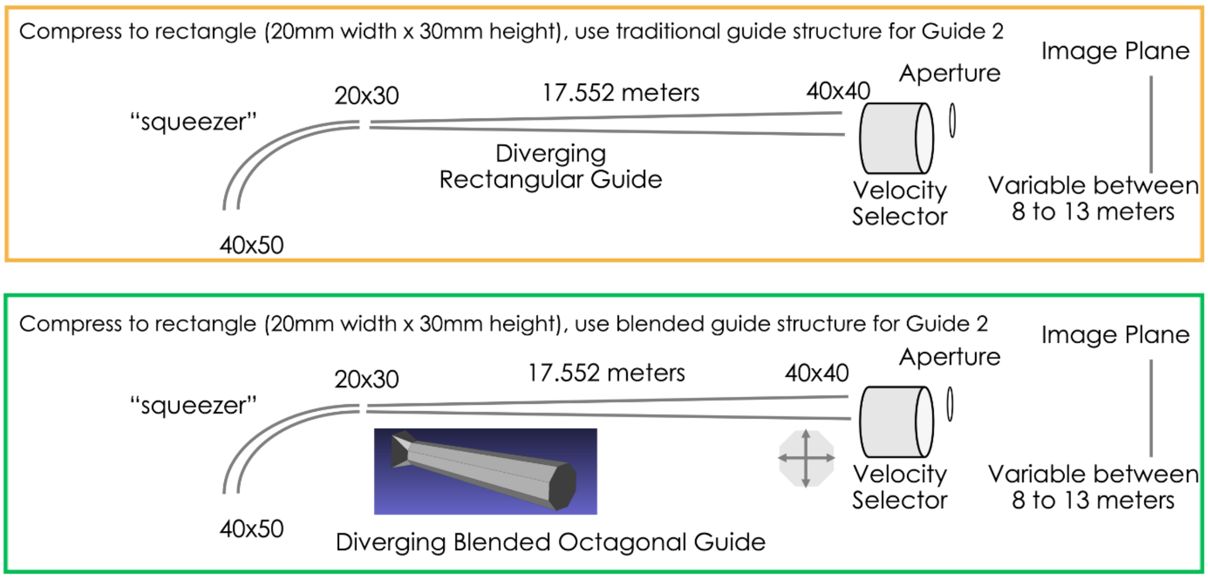
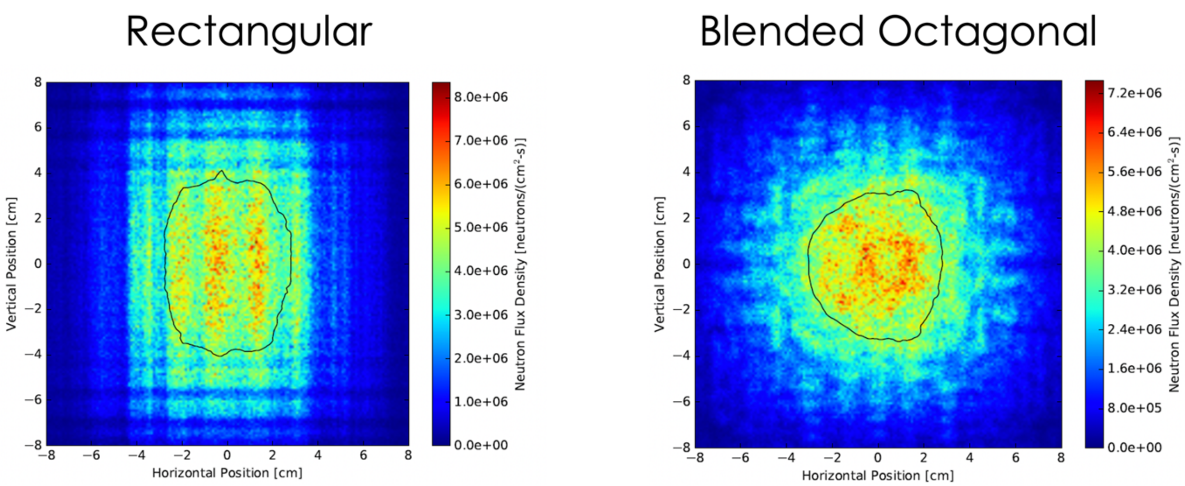



**Figure 31. NB-4 Conceptual IMAGING beamline layouts that were studied in McStas.**

The simulations included a calculation of a radiograph at the detector plane for a specific *L/D* ratio, without a diffuser in the beam path, and histograms of the divergence profiles (horizontally and vertically) at the guide exit. In addition to optimizing flux on sample for a given setting, these metrics (pinhole image and divergence profile) should show a beam that is as homogeneous as possible. An additional quantity derived from the simulated radiographs was the area of the FOV as defined in the requirements (the local intensity does not drop below 75% of the maximum). A 1 cm smoothing box filter was applied in the process of making the FOV calculation. This approach was found to be the right compromise between accuracy and smoothness of the contour lines. All intensity numbers in Figures 32–37 are for a white beam, integrating between 1 Å and 6 Å.

Again, it can be concluded that a conceptual design based on a traditional rectangular guide can be chosen. Such a design fares better with regard to intensity, and the local inhomogeneities in the images are not fundamentally better if an octagonal guide is chosen.

The analysis of the *m*-values of the guide coating is preliminary at this time and remains to be finalized. A final design of the beam transport system for this instrument will perhaps include a focusing guide end section with an exit size matching the maximum *D* value at which the instrument is to operate, around 2 cm. This work remains to be done.




| Guide Shape | 75% Level Integral | 75% Level Area | Smoothed Max Flux |
|---|---|---|---|
| Rectangle | 1.35e8 n/s (1-6 Å) | 36.2 $cm^2$ | 4.29e6 n/($cm^2$-s) (1-6 Å) |
| Octagon | 1.07e8 n/s(1-6 Å) | 30.1 $cm^2$ | 4.25e6 n/($cm^2$-s) (1-6 Å) |

**Figure 32. Radiograph at the detector plane simulated at NB-4 (empty beam, no sample) with high resolution (L/D=1,740).** The black contour lines represent the area where the local intensity is >75% of the maximum. This is integrating over the spectrum between 1 Å and 6 Å.

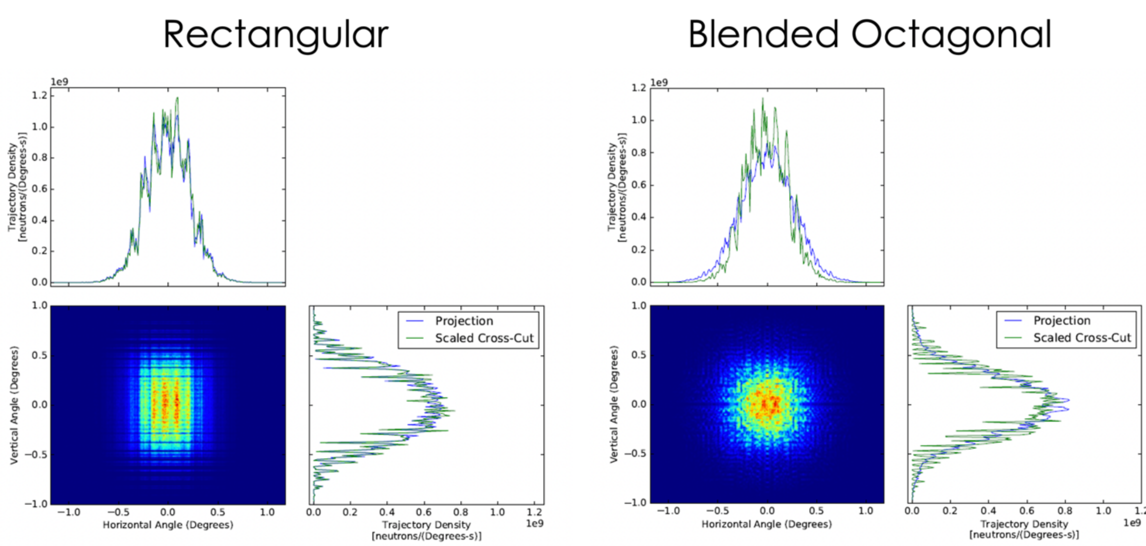
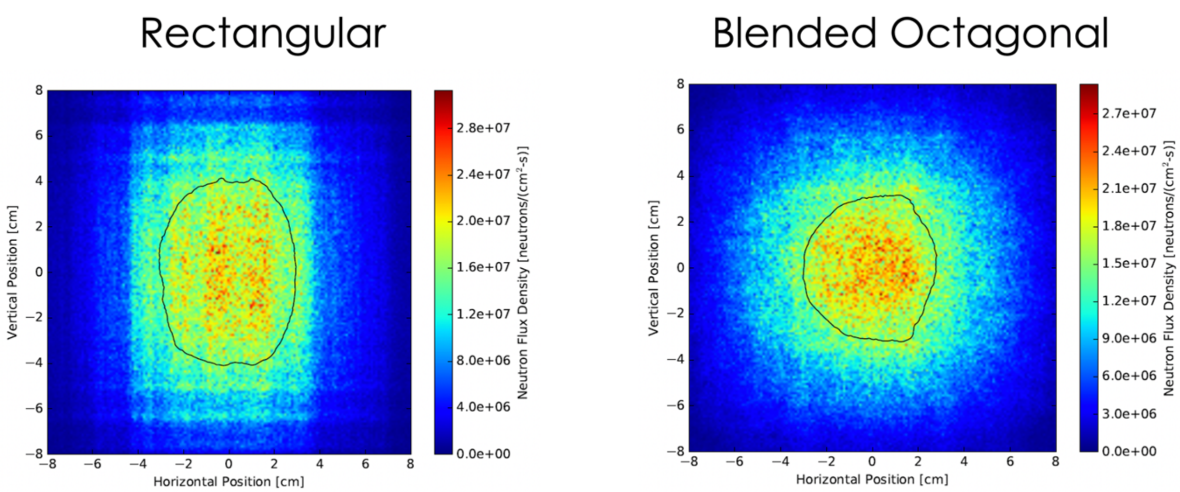



**Figure 33. Guide exit divergence maps at NB-4 with high resolution (L/D=1,740).** This is integrating over the entire white spectrum between 1 Å and 6 Å. The blue traces are integrating over the entire area whereas the green traces go through the center of the area.




| Guide Shape | 75% Level Integral | 75% Level Area | Smoothed Max Flux Density |
|---|---|---|---|
| Rectangle | 5.86e8 n/s (1-6 Å) | 40.3 $cm^2$ | 1.65e7 n/($cm^2$-s) (1-6 Å) |
| Octagon | 4.11e8 n/s (1-6 Å) | 28.9 $cm^2$ | 1.62e7 n/($cm^2$-s) (1-6 Å) |

**Figure 34. Radiograph at the detector plane simulated at NB-4 (empty beam, no sample) with medium resolution (L/D=870).** The black contour lines represent the area where the local intensity is >75% of the maximum. This is integrating over the spectrum between 1 Å and 6 Å.

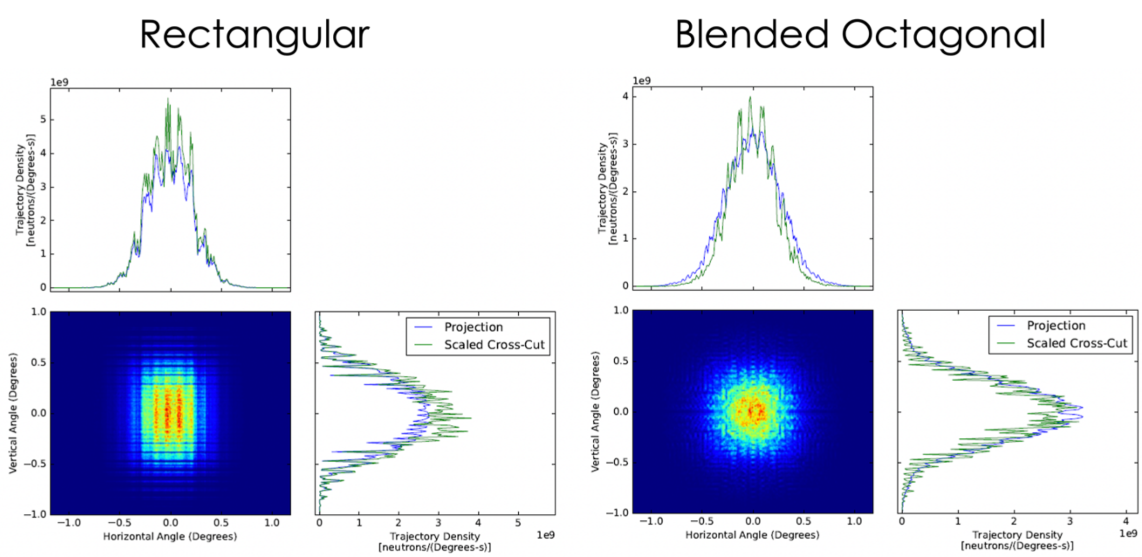
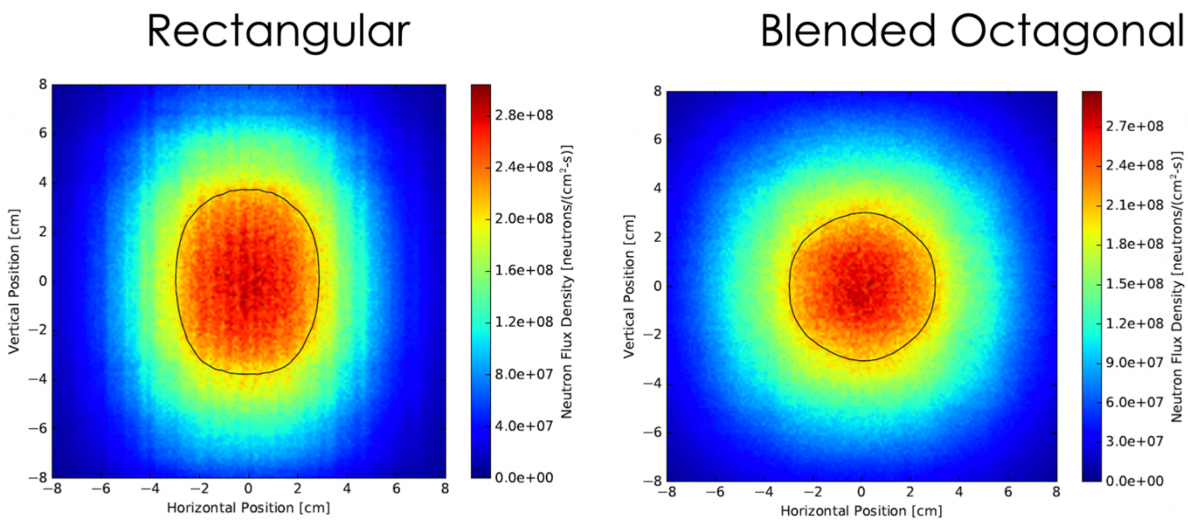



**Figure 35. Guide exit divergence maps at NB-4 with medium resolution (L/D=870).** This is integrating over the entire white spectrum between 1 Å and 6 Å. The blue traces are integrating over the entire area whereas the green traces go through the center of the area.




| Guide Shape | 75% Level Integral | 75% Level Area | Smoothed Max Flux Density |
|---|---|---|---|
| Rectangle | 7.11e9 n/s | 36.0 cm$^2$ | 2.23e8 n/(cm$^2$-s) |
| Octagon | 5.32e9 n/s | 28.4 cm$^2$ | 2.15e8 n/(cm$^2$-s) |

**Figure 36. Radiograph at the detector plane simulated at NB-4 (empty beam, no sample) with low resolution (L/D=230).** The black contour lines represent the area where the local intensity is >75% of the maximum. This is integrating over the spectrum between 1 Å and 6 Å.

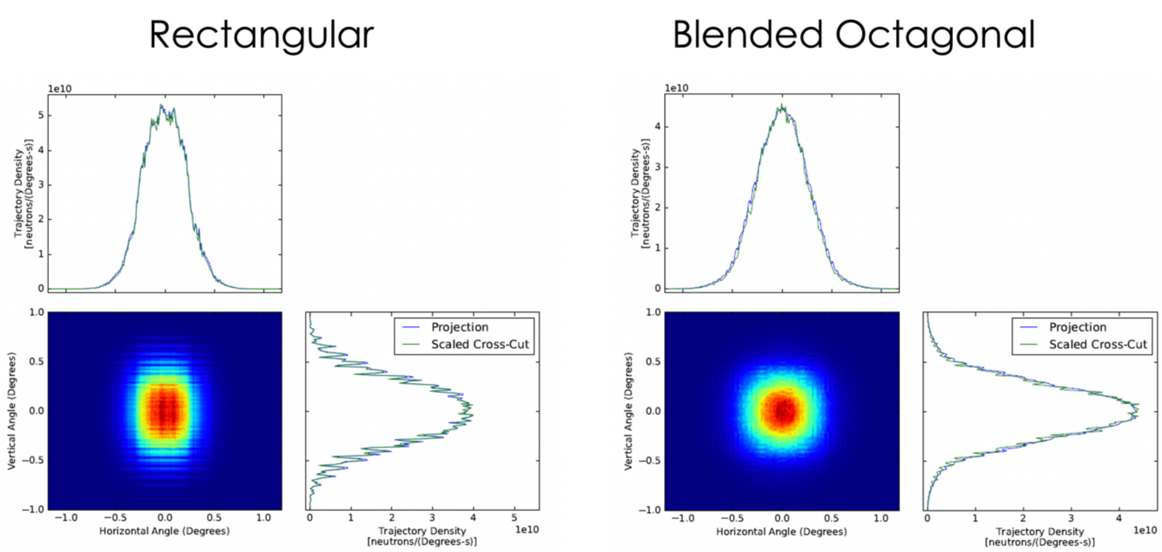



**Figure 37. Guide exit divergence maps at NB-4 with low resolution (L/D=230).** This is integrating over the entire white spectrum between 1 Å and 6 Å. The blue traces are integrating over the entire area whereas the green traces go through the center of the area.

### 4.6 NB-5 GP-SANS

Given the space constraints to the east (MANTA at NB-6) and west (IMAGING at NB-4), the biggest change to the GP-SANS beamline will be relocation by approximately 3.5 m downstream. There are two main reasons for making the change: to improve the crane coverage above the GP-SANS sample area and to allow more space for the MANTA secondary spectrometer at NB-6. The proposed move downstream of the vacuum tank is far enough that the current footprint of the guide hall cannot accommodate it without modifications to the building.

The optimization of the new GP-SANS beam transport was constrained by the location of the sample and the direction of the beam at that point. Since the GP-SANS tank is in a trench, moving the tank sideways would present significant additional logistical difficulties.

The GP-SANS beam changes direction between the HB-4 beam tube and the sample position, but much less so than the other beamlines. It is the least curved beam in the HFIR guide hall. The alternatives considered to achieve the bend were an optical filter and a true curved section (bender) with and without septa. Given the space constraints, the optical filter was found to be the best solution. There was no solution for a truly curved guide that would line up the beam direction at the sample position with the current direction.

The permanently installed neutron guide stops short of the sample position by some 18 m. The primary way in which the instrumental Q resolution is changed is the introduction of additional (between 0 and 8) short sections of guide between the permanent guide exit and the sample. This is exactly the same concept as at Bio-SANS. These short sections are indicated in blue in Figure 38. They enable the transport of a higher divergence to the sample, for more flux at the expense of Q resolution.

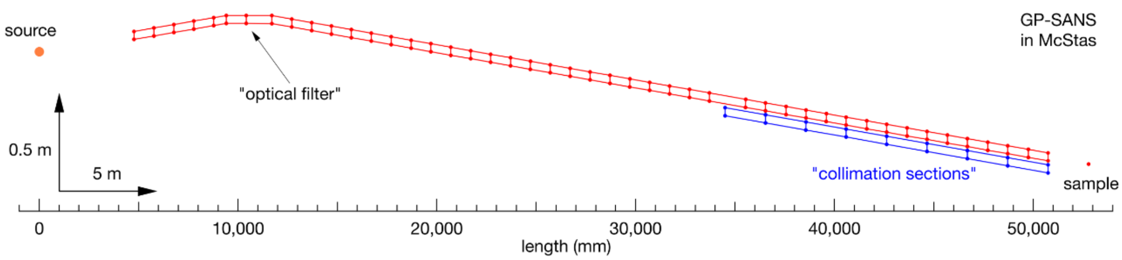



**Figure 38. GP-SANS model in McStas.**

Individual sections of guide are modeled in McStas with 1 m long straight tiles of glass.

Besides the question of how to realize the necessary change of direction in the guide, the bulk of the optimization work for GP-SANS concerned the *m*-values of the guide. In the absence of a velocity selector, the optimization sought to maximize the number of “good” neutrons at the sample position with wavelengths of $\lambda > 4$ Å, while minimizing the number of “bad” neutrons with wavelengths of $\lambda < 3$ Å. The result showed that it is best to leave the *m*-values throughout the guide unchanged at $m=1$, with the exception of the “optical filter” outer surface, at which $m=3$ should be selected.

It was also found that the guide entrance should be illuminated with the “natural” divergence at this point; that is, no neutrons bouncing off other surfaces (for example, in the collimator in the HB-4 beam tube) should make it into the guide. See Figures 39 through 42.

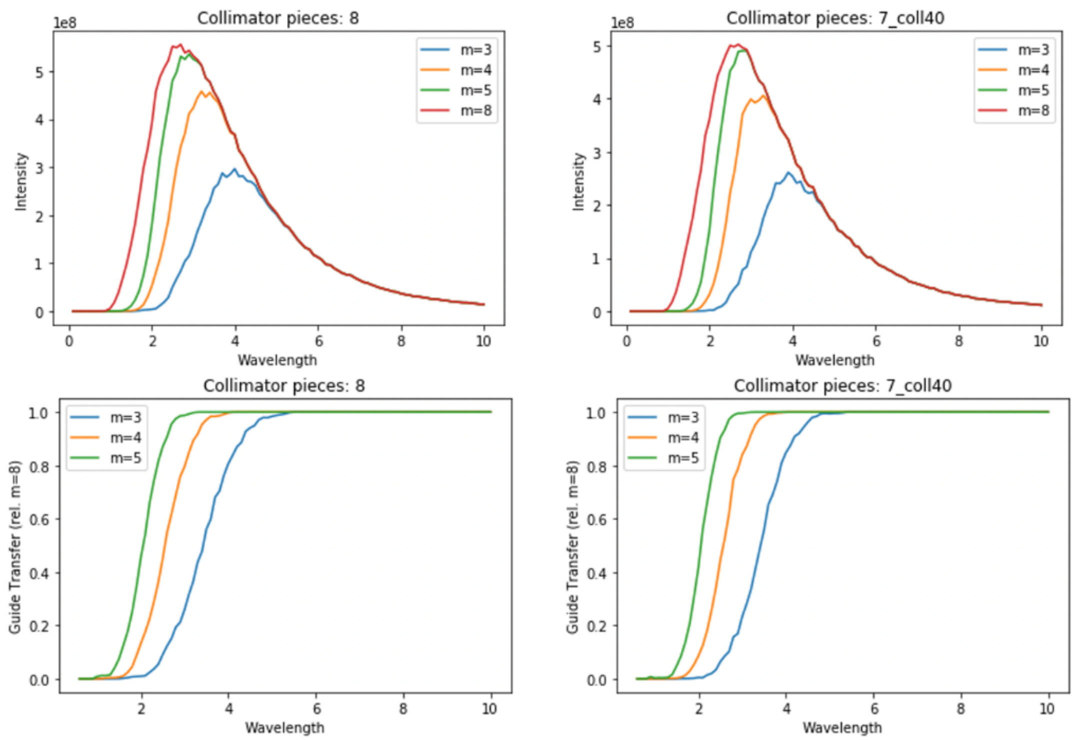



**Figure 39. GP-SANS spectra at the sample position, calculated with McStas, with various choices for the m-value in the optical filter and the number of guides instead of collimation (8 is the maximum).**

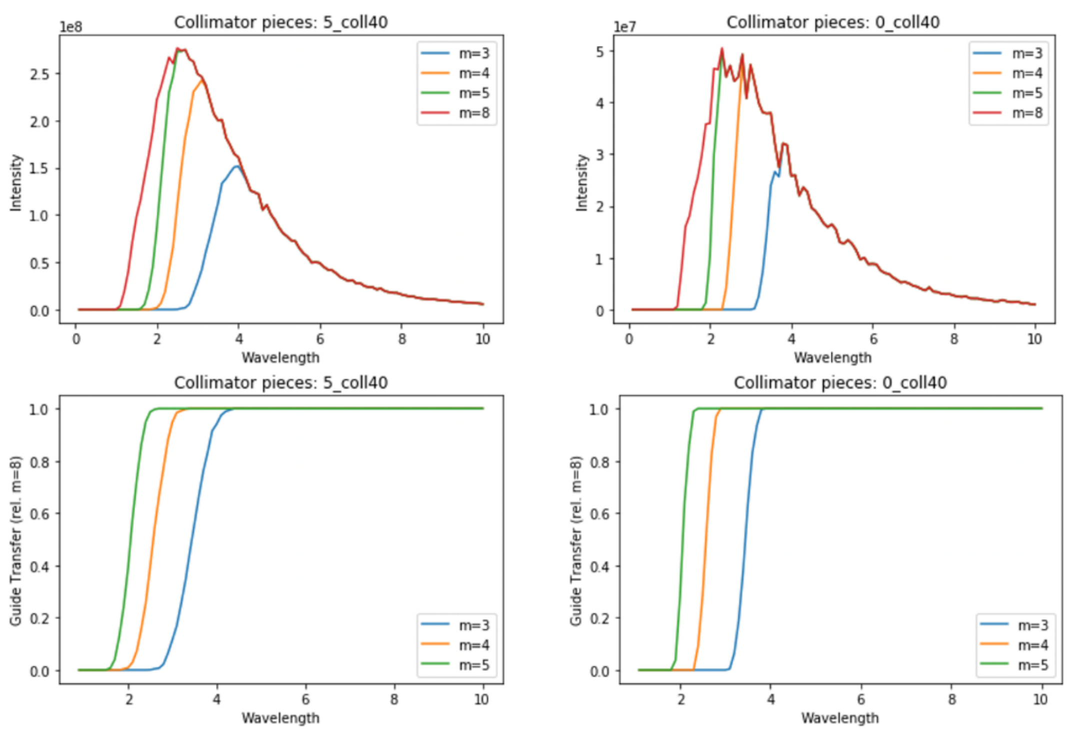



**Figure 40. GP-SANS spectra at the sample position, calculated with McStas, with various choices for the m-value in the optical filter and the number of guides instead of collimation (8 is the maximum).**

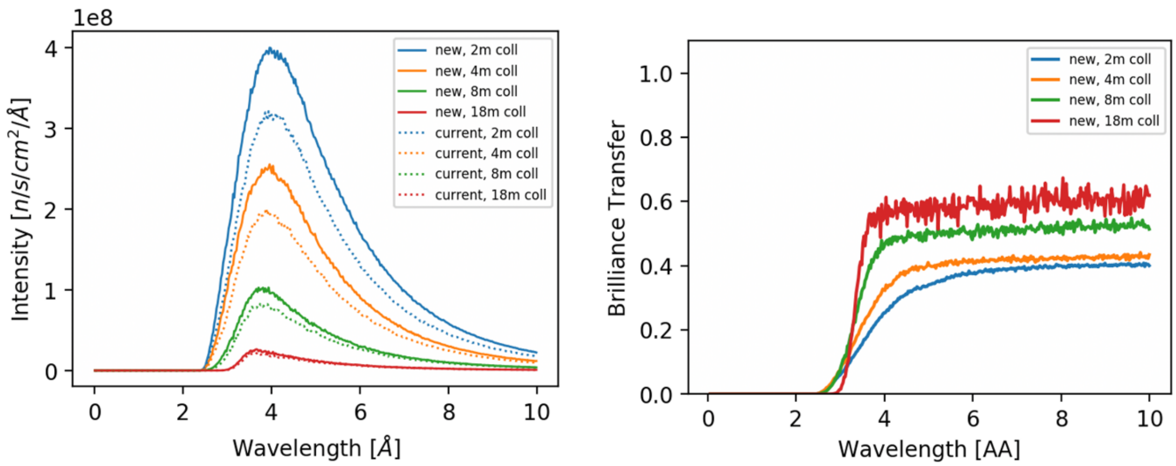



**Figure 41. GP-SANS spectra (left), for collimation lengths between 2 m and 18 m, showing a direct comparison between the existing and the proposed new instrument design.** The image at right shows the brilliance transfer. All these data are taken at a 2 cm diameter sample with the horizontal divergence at the sample position shown in Figure 43.

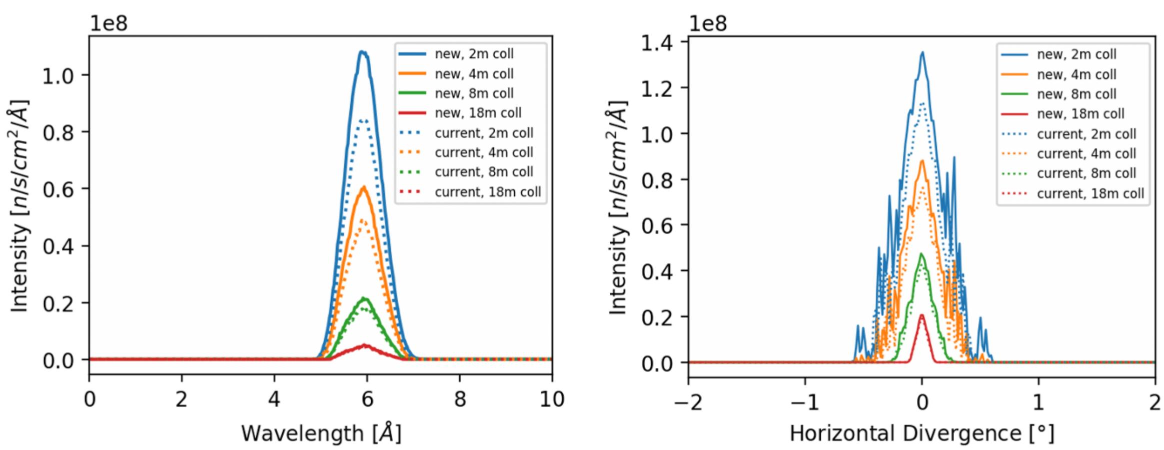



**Figure 42. GP-SANS spectra (left) through a velocity selector set to run at 6 Å, and horizontal divergence at the sample position.** The vertical divergence is similar but smoother, the beam dimensions at the guide exit and at the sample position are the same vertically and horizontally.

Figure 43 and Figure 44 show the illumination of a 2 cm sample disk, depending on the collimation length.

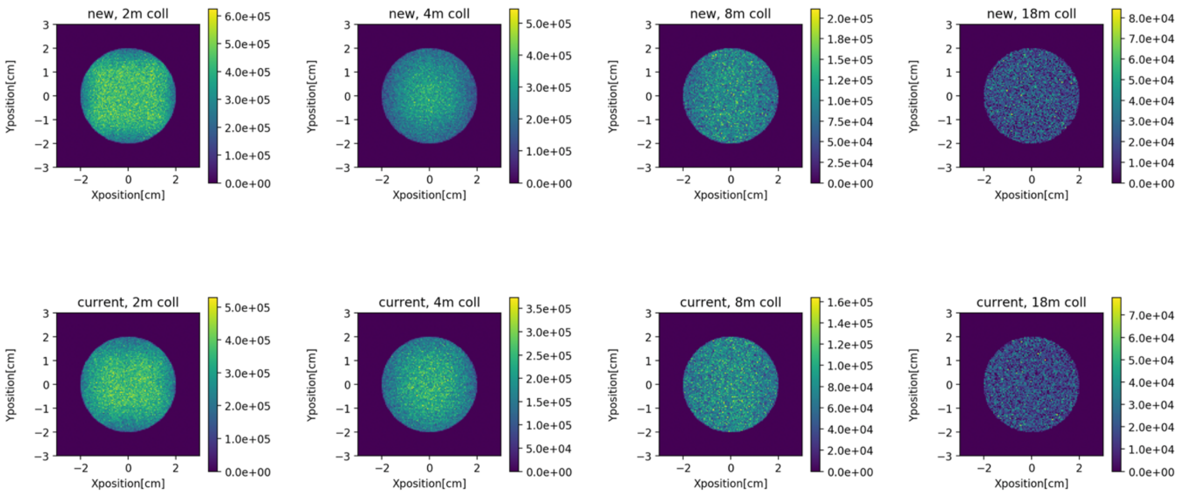



**Figure 43. Sample illumination at GP-SANS with various collimation lengths.**

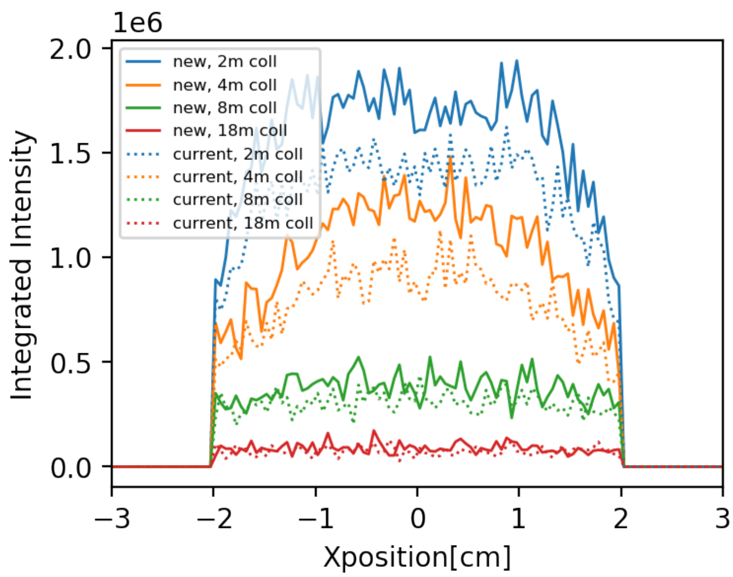



**Figure 44. Horizontal cut through the sample areas shown in Figure 43.** The sample scattering was simulated with McStas in the same way it was calculated for Bio-SANS, this is shown in Figure 45.

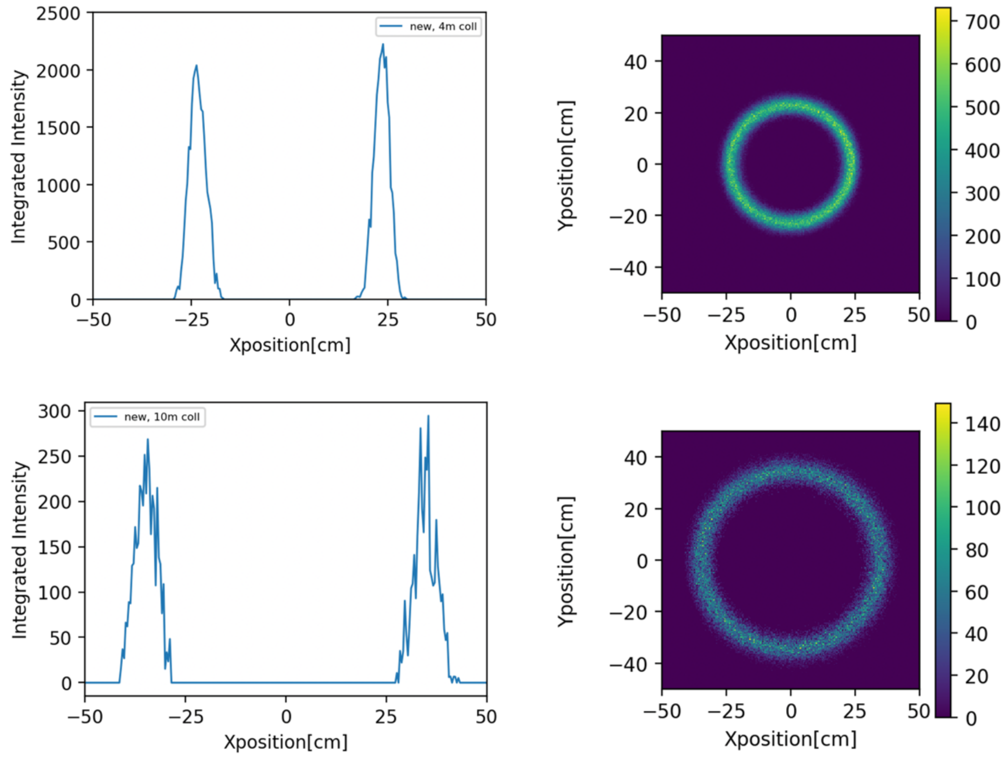



**Figure 45. Scattering from a sample in the high intensity case (upper row, powder with d=58 Å) and in the high resolution case (lower row, powder with d=120 Å).** The powder rings are on the right-hand side, horizontal cuts through the data are on the left-hand side.

In summary, the results for GP-SANS show a modest performance gain of ~30% over the existing installation, due mainly to the reduced distance (from ~5 m to ~4 m) of the guide entrance to the source.

## 4.7 NB-6 MANTA

MANTA is envisioned to be a double-focusing triple-axis spectrometer with a multi-analyzer back end. This section summarizes the guide that will transport neutrons to the monochromator. The design has many constraints, which are described first.

Though the design is yet to be optimized, a 30×30 $cm^2$ monochromator was assumed to help define constraints. In the horizontal direction, the monochromator will be of a symmetric Rowland focusing design with a 1.4 m focal length. This length, and the assumption of 70 cm of shielding around the incident beam, limit $E_i$ to greater than 2.4 meV. Furthermore, the size of the building and the size of the secondary spectrometer location restrict where the sample can be positioned. Specifically, we assume a multi-analyzer design, similar to the CAMEA [4] design, with 1 m of clearance behind it for equipment movement. This assumption, combined with the aforementioned monochromator focusing length, fixes the monochromator position along the beamline at 28.133 m along a line from the source, offset by 0.985 m in the horizontal and 0.153 m in the vertical.

Perpendicular to the beamline in both directions (horizontally and vertically), it is constrained by existing openings such as the bulkhead pass-throughs in the reactor confinement building wall, which cannot be changed. Before entering the Cold Guide Hall, the neutron guide is horizontally curved to avoid line-of-sight to the source. Entering the guide hall, a straight section follows (the “randomizer” in Figure 46) to re-center the flux. The curved section was constructed using a logarithmic spiral formalism of equal angle tilts for segments of varying lengths, with the constraint of being in line with the shutter guide section. Nevertheless, the guide is circular to within manufacturing tolerances, with a radius of curvature of 348.735 m. The maximum width of the guide is constrained by the maximum width of the elliptical focusing optic, which is described below. The curved section has three channels, and all surfaces of the supermirrors are coated with *m*=3.

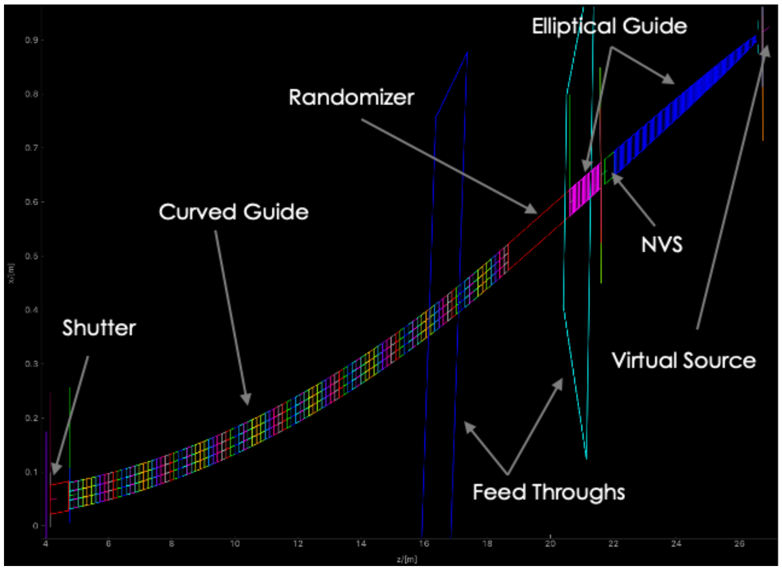



**Figure 46. The MANTA horizontal guide configuration.**

Inside the Cold Guide Hall, a neutron velocity selector (NVS) will be located 405.4 mm (16 in.) downstream of the wall of the hall, and a place for a 125 mm thick secondary shutter is located on its upstream side. The NVS will be 306 mm long and have a beam path 45 mm wide and 135 mm tall.

In the horizontal direction, a focusing optic, consisting of a half ellipse, will begin as soon as the guide enters the guide hall building (downstream of the randomizer). The beam will be 48.6 mm wide at this point, equal to the minor axis of the ellipse. The shape of the ellipse will be determined by locating the focal point 1.4 m upstream of the monochromator to create a virtual source for the Rowland focusing principle. The ellipse width will be smaller than the width of the NVS to reduce loss from this component. Another effect of the randomizer is that it will minimize the coupling between the downstream focusing optic and the upstream curved section. The required length of the straight section, the monochromator position, and the use of the half-ellipse shape will set the guide width at the start of the ellipse to 48.6 mm wide.

The performance of the ellipse is demonstrated in Figure 47, which shows a horizontal cut across the sample spot. Roughly double the flux is provided compared with a straight guide. The impact of the gap in the guide for the velocity selector will be comparatively minor. Figure 47 shows that using elliptical focusing to the virtual source works better for the Rowland focusing geometry than does no focusing. It also shows that placing the NVS in a location where the divergence is relatively small has little (if any) bad effect on the flux on sample.

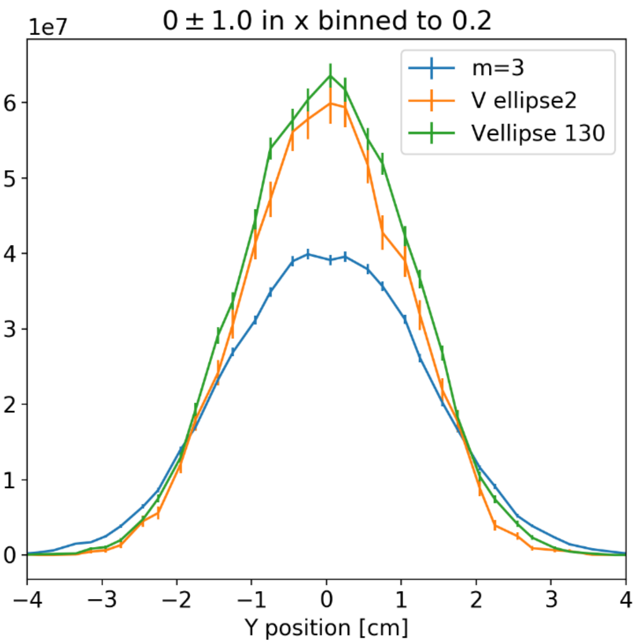



**Figure 47. The impact of the elliptical focusing section, compared with a simple, straight, and non-focusing section.** This figure shows a horizontal intensity cut through the sample position with a vertical integration range of ±1 cm.

In the vertical direction, see Figure 48, the guide will expand the beam only very slightly to reduce the divergence on the monochromator. This will provide a better-collimated beam and thus a more focused beam. The direct path in the vertical will point upward by 0.28°, and the monochromator will be used to move the focusing spot down so that the beam on the sample table will be horizontal.

Overall, the beam transport is expected to provide 1.13(3)×$10^8$ n/cm$^2$/s at $E_i$=5 meV on the sample, a gain factor of more than 30 over the current installation at C-TAX. The beam spot size and shape are summarized in Figure 49.

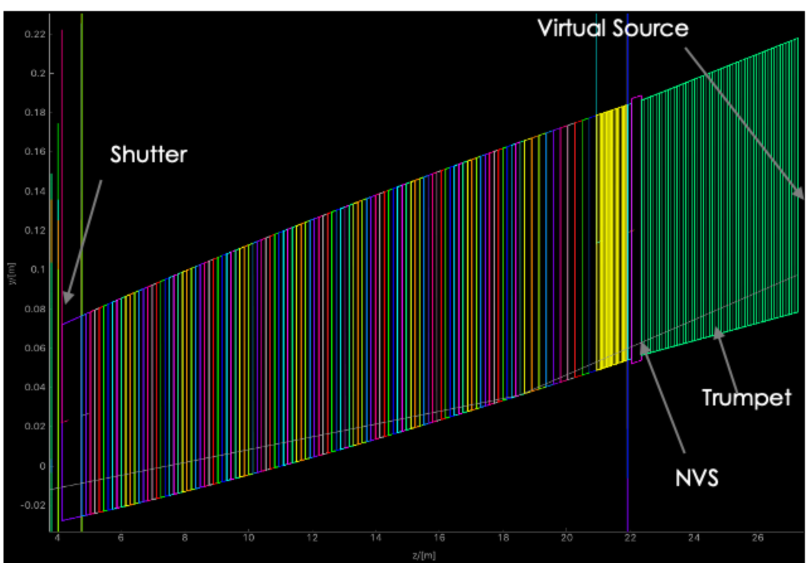



**Figure 48. The MANTA vertical guide configuration.**

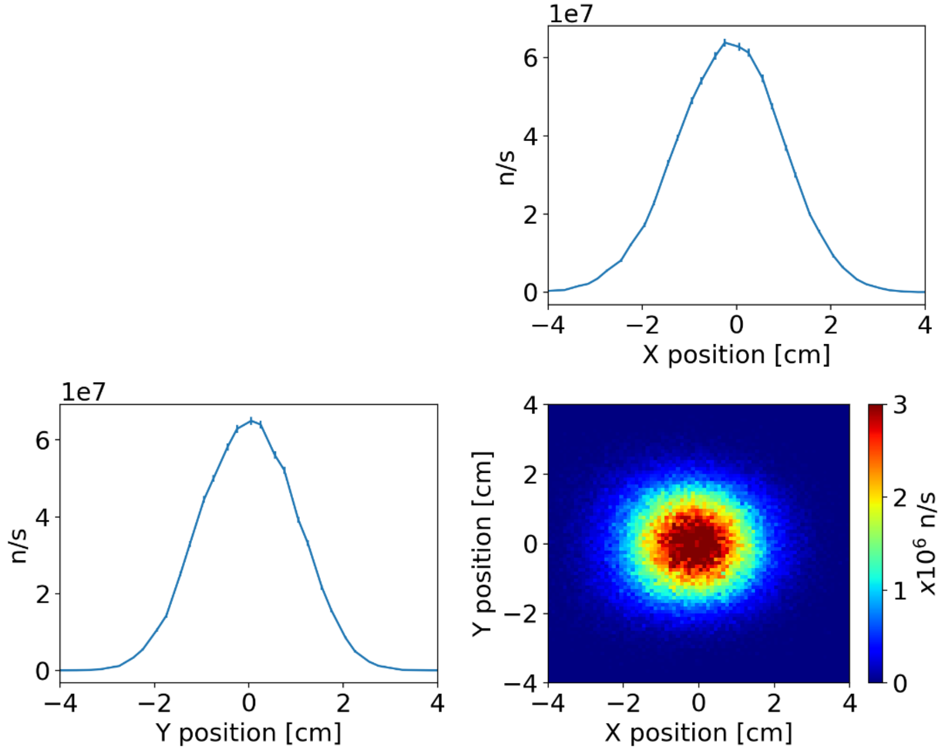



**Figure 49. Beam spot at the sample position for 5 meV neutrons.**

# 5. SUMMARY AND CONCLUSIONS

This report presents the design of a replacement cold neutron guide system for HFIR. The guide system is being redesigned at this time because a rare opportunity for a major upgrade and renewal presents itself with the necessary beryllium reflector replacement and the associated temporary facility shutdown in 2024–2025. The possible changes are bounded by a number of site and operational constraints, but the instruments still are expected to gain in their flux on sample by a factor of between 1.3 and 3. An exception is the C-TAX instrument, which stands to gain a factor of >30 in flux at the sample. The new guide system will also offer additional performance gains, such as an increase in Q-range on Bio-SANS.

The proposed new guide system requires an expansion of the Cold Guide Hall to the south by approximately 4,200 sq. ft. This is the only direction in which the building can be expanded to make more room for instruments and equipment.

The redesign of the neutron beam transport systems was guided by scientific requirements for the individual beamlines and by high-level facility goals, which were formulated based on advice from an external advisory committee. The high-level goals are

1. Add a new spin echo neutron spectrometer to the cold neutron instrument suite.

2. Increase the number of guides from four to six so that every instrument can be on an end-guide position.

3. Improve instrument performance where possible.

4. Ensure that after the guide reconfiguration, every instrument performs at least as well as it currently does.

The design of the guide system in the common sections up to about 25 m from the source is considered to be complete and ready for engineering design, whereas the designs of the instrument-specific guides is still in progress in some cases.

The improved design of the guide network, and the resulting performance values for the individual instruments, will help to ensure long-lasting success for the scientific user program going forward. With the addition of a spin echo instrument, the cold instrument suite at HFIR will be a good complement to the SNS, making optimal use of the intense time-averaged brightness of the HFIR cold source.

# 6. REFERENCES

[1] Dan Neumann et al, *Report of the ORNL Neutron Sciences Instrument Advisory Board*, report of the January–25, 2018, meeting, 2018. (The report is included as Appendix A).

[2] P. Willendrup, E. Farhi E. Knudsen, U. Filges, and K. Lefmann, *Journal of Neutron Research*, 17(1), 35–43, 2014, DOI 10.3233/JNR-130004.

[3] J. L. Robertson and E. B. Iverson, Neutron News **19**, 17-19 (2008).

[4] Felix Groitl, Dieter Graf, Jonas Okkels Birk, Márton Markó, Marek Bartkowiak, Uwe Filges, Christof Niedermayer, Christian Rüegg, and Henrik M. Rønnow, "CAMEA—A novel multiplexing analyzer for neutron spectroscopy," *Rev. Sci. Instrum.* 87, 035109 (2016), https://doi.org/10.1063/1.4943208

# APPENDIX A. REPORT OF THE ORNL NEUTRON SCIENCES INSTRUMENT ADVISORY BOARD, JANUARY 24 AND 25, 2018

## Summary

The Instrument Advisory Board (IAB) of ORNL Neutron Sciences Directorate met on January 24-25, 2018 to discuss future neutron instrumentation at ORNL over the next 10 to 15 years. ORNL currently operates two neutron sources, the First Target Station (FTS) at the SNS which provides intense pulsed neutron beams optimized for short pulses and thermal neutrons, and the High-Flux Isotope Reactor (HFIR) which provides high time-averaged brightness of both cold and thermal neutrons. Instrumentation at these sources provides excellent capabilities for a broad range of scientific applications.

Over the next dozen years or so, ORNL expects to build and commission a second target station (STS) at the SNS which will be optimized for cold neutrons and high brightness. The IAB was excited to hear about the recent progress that has been made in designing very bright parahydrogen moderators for the STS. The ability to examine a scale model of the STS target/moderator system was also illuminating. The new moderators provide fresh opportunities to optimize instrumentation across the three sources (FTS, STS and HFIR) and exploit their complementary capabilities. ORNL must also coordinate further improvements to their existing instruments with the construction of new instruments across their three sources. It is important that ORNL proceed with a holistic approach that optimizes the placement of new instruments across these sources to maximize their overall neutron scattering capabilities and scientific impact now and into the future.

This report summarizes the IAB's discussions and provides suggestions for future instrumentation at ORNL. The key assumptions of this report are:

a) the STS will be completed (or nearing completion) at the end of this time frame;

b) HFIR will operate throughout this period, except for a year-long outage to replace the Be reflector, and will continue for a significant period into the future;

c) the First Target Station (FTS) at SNS will continue operations throughout this period.

This set of assumptions is referred to as the "three source vision" for neutrons at ORNL. If any of these assumptions are not met, our advice would be altered.

Just as importantly, the final optimization will require detailed simulations of the way instruments perform at each of these three sources. This means that final decisions about the instrument suite cannot yet be made definitively. This meeting of the IAB was very timely because the board could discuss a broad range of issues and provide input during the decision-making process. Thus, the input in this report should be taken as part of the evolving optimization process: as simulations are performed our advice might indeed change. With these caveats, the following recommendations are in our priority order.

1) *The IAB recommends that ORNL add new instruments to the FTS.* The imaging station, VENUS, should have the highest priority. An imaging station would likely help ORNL better engage industry and would provide a large field of view and energy resolved capability unmatched in the US. The nation is also in need of more capacity and enhanced capabilities for neutron powder diffraction, both for traditional Rietveld refinement and for pair distribution function (PDF) analysis. Thus, the committee believes that the two additional powder diffractometers, DISCOVER and HiResPD, should also be built at FTS with high priority. The combination of these two instruments would round out the powder diffraction suite. Moreover, these instruments fit extremely well into the three source

vision providing capabilities on the first target station that would not be superseded by the performance of instruments at the STS. We realize that the construction of HiResPD requires relocating instruments and the IAB sees no disadvantages with the proposed moves. We believe that it is essential that this be done as soon as possible.

While the three-source vision appears to be well developed for the operation and development of FTS within the context of STS, the role of HFIR within this context was less clearly articulated. *The IAB believes that ORNL must deliver an impactful and sustainable plan for HFIR that exploits its high time averaged cold and thermal brightness.* ORNL should balance the entire instrument suite across all three sources as well as the capabilities at NIST. We acknowledge the complexity of optimizing such diverse opportunities across the sources, and emphasize that rational choices cannot be made without detailed simulations.

1) The IAB recommends that ORNL update and optimize the thermal neutron instrument suite at HFIR to provide the US neutron community with internationally competitive instrumentation. The HFIR thermal brightness will not be superseded by either FTS or STS. Thus, providing the US scientific community with state-of-the-art thermal neutron capabilities at HFIR is essential to effectively realizing the three-source vision. In light of these considerations, ORNL must develop and implement a renewal plan for the outdated thermal instrumentation at HFIR.

2) The IAB recommends that ORNL finalize plans for upgrading the cold neutron delivery system at HFIR. The cold source at HFIR is very bright. Unfortunately, the geometry of the HB4 tube where the cold source is located imposes severe geometrical challenges on the efficient transfer of large numbers of neutrons to the guide hall. Thus, this source is ideally suited for instruments where brightness is the primary consideration e.g. SANS and neutron spin echo (NSE). The IAB agrees that ORNL must take advantage of the replacement of the Be reflector as an opportunity to improve the delivery of cold neutrons. As part of this upgrade, ORNL should enhance the cold neutron instrumentation at HFIR.

    a) *The IAB recommends that ORNL develop a national roadmap for NSE.* The US scientific community lacks access to an NSE instrument capable of measuring the same range of time scales as IN15 at the ILL, placing them at a significant disadvantage. ORNL has stated that they don't currently have the expertise to build an NSE and that they will begin to gain that expertise when the FTS NSE is transferred from Jülich to ORNL two years from now. The IAB feels that this approach is too casual for an instrument that has been repeatedly identified as a high priority by the US scientific community. Providing such a capability in the US will be a major undertaking which requires substantial contributions from international experts. This should be informed by the previous workshops and the three source vision.

    b) *The IAB believes that ORNL should develop a modern guide and the primary spectrometer for a new cold triple-axis spectrometer.* The cold triple axis, CTAX, has long suffered from poor neutron transport from the cold source and urgently needs to be upgraded. We recommend that ORNL should initially use the secondary spectrometer from CTAX. The instrument should be compatible with Larmor precession methods. MANTA is consistent with the three source vision as it is unlikely that the capabilities of this instrument will be superseded by STS.

    c) *The IAB believes that the new cold guide system should not degrade the performance of the cold imaging station and should enhance it if possible.* Neutron imaging also relies largely on brightness, though field of view is also an important consideration. Alternatively, the cross-source optimization could result in this instrument being relocated to a thermal neutron beam after the Be-reflector outage.

d) *The IAB believes that ORNL should NOT build a new SANS in the HFIR cold guide hall.* While the IAB believes SANS is important, an additional SANS is not essential in the national context. Already 20% of the neutron scattering instruments in the US are SANS machines and thus this would only increment that SANS capacity slightly. Rather, ORNL should consider building two new SANS instruments at the STS one of which should be something like SWANS. The IAB believes that this is a better option than building a third SANS instrument in the cold neutron guide hall that would be moved to the STS when complete, providing only a few years of operation at HFIR. It is not clear how this would advance the three source vision and the resources that would go into moving the instrument would be better spent elsewhere.

The instruments outlined as high priority concepts for STS appear to be appropriate to the new source and have a good level of technical and scientific ambition. *The IAB encourages the continued development of these STS concepts and to further explore possibilities such as a 2nd SANS, an imaging station, a cold version of HIGGS and a WISH-style diffractometer.* Further detailed simulations of the instrument performance should be pursued to inform any movement of instruments from FTS to STS and from HFIR to STS. Though the IAB cautions that moving instruments between sources should be pursued sparingly and only where there is a substantial performance enhancement. Wolter optics promise a way to effectively focus polychromatic neutron beams. As they would work particularly well for cold neutrons, the IAB believes ORNL should be working with NASA and NIST to advance this technology for use, particularly at STS.

**I) ORNL Neutron Sources 2030, source profiles and instrument suites:**

a) Do the characteristics of HFIR, FTS, and STS complement each other in a way that allows optimal placement of instruments and neutron scattering techniques?

The three neutron sources have very different characteristics which can be used to provide distinct and complementary capabilities. Here we describe the source characteristics and make suggestions as to how these can be exploited to provide the US scientific community access to a broad range of world-class neutron capabilities.

**High Flux Isotope Reactor (HFIR)**

Currently HFIR has roughly equal numbers of thermal and cold instruments, with the thermal instruments distributed on three beam-ports, and the cold instruments viewing a horizontal cold source. The time-average brightness of the thermal beam tubes exceeds that of the FTS and STS moderators by more than an order of magnitude. This translates into a strong potential for high-performance instrumentation, using focusing crystal monochromators. Fulfilling this potential requires a dramatic modernization of the existing suite of thermal instruments, prioritizing quality over the number of instruments, and bringing the remaining instruments up to the state-of-the-art at other facilities. This will involve upgraded monochromators, detectors, and shielding, along with careful simulation-based optimization. The large-area beam-tubes and best-in-class time-average brightness present a potential opportunity for thermal imaging which should be studied as part of developing a holistic approach to neutron imaging at ORNL and within the US community.

The time-averaged brightness of the cold source at HFIR exceeds that of the STS moderators by about a factor of two and of the FTS coupled moderator by about an order of magnitude. HFIR thus provides opportunities for world-class cold neutron instrumentation. However, the performance of the cold instruments at HFIR is compromised by the beam extraction arrangement, in which a rather small cold source is viewed by a guide system starting at 5 m. The proposed reduction of this distance to 4 m will improve the situation, but the cold guides will still be significantly under-illuminated for many applications. In addition, the large number of guides means that each is rather small, thus hindering the performance for many applications. The highest performance can therefore be found for instruments that rely primarily on brightness, such as SANS and neutron spin echo. To enhance the instrumentation at HFIR, potential increases in cold source brightness and further significant reduction in the moderator-guide distance should be studied. Taken together, these could dramatically increase the cold-neutron performance, particularly for instruments which require large phase space volumes such as triple-axis instruments with large double-focusing monochromators.

Finally, HFIR should exploit the comparative simplicity of monochromatic instruments for polarized-neutron applications, such as spherical polarimetry and novel precession techniques.

**SNS First Target Station (FTS)**

The FTS has a mature suite of instruments which are well-suited to its source characteristics. Once the STS comes online, a small number of instruments should be considered for relocation to the STS to benefit from the excellent cold neutron performance that source. The IAB recommends that when new instruments are built at the FTS over the coming years, a view is maintained of the expected STS parameters, so that the new instruments do not end up having to be relocated. It is clear, however, the FTS will remain a very attractive option and will continue to be the source of choice for many applications.

The decoupled and poisoned moderators provide pulse widths which are better-suited to high-resolution applications. That is the case both for thermal/epithermal neutrons where the water moderators provide significantly sharper pulse widths than the STS moderators, as well as for the cold moderators, where the pulse width can be up to an order of magnitude less at long wavelengths. Since very long flight paths are not available at the STS, these short pulse widths are the only means of reaching the high wavelength resolution needed for high-resolution spectroscopy and diffraction.

While the peak brightness of the FTS and STS moderators are very similar for neutron energies above about 100 meV, the higher repetition rate of the FTS provides a significant gain at these energies.

The viewed moderator surface at the FTS is typically of the order of 100 $cm^2$ or more. This further enhances the performance of instruments using epithermal neutrons where guide transport is less effective, allowing short instruments to let the moderator illuminate the sample directly, while still delivering a sufficient beam divergence to reach the required high flux at the sample. Similarly, an imaging instrument placed at the FTS can view the moderator directly, without using a neutron guide. This will provide a very uniform illumination of a relatively large field of view, minimizing systematic errors arising from the unavoidable beam divergence structure associated with reflective neutron optics.

**SNS Second Target Station (STS)**

The STS will be the world leader for peak cold neutron brightness, a key parameter for high wavelength resolution neutron scattering instruments. Of the three sources, it will also provide the highest peak brightness of thermal neutrons. It will therefore be the source of choice for many neutron instruments.

The increased peak brightness of the STS will be game-changing for many cold neutron applications. It will be an excellent source for reflectometry, medium-resolution spectroscopy, and high-intensity instruments that require only moderate wavelength resolution, such as SANS and spin echo.

The high source brightness is achieved partly by reducing the viewed size of the source, which lends itself to producing small, intense beam spots. This is perfectly suited to measuring small samples, or small parts of larger, sometimes inhomogeneous sample.

The very fast measurement times enabled by the high peak brightness will allow systems to be studied which vary on the second-to-millisecond timescale.

The 15 Hz repetition period will result in a large bandwidth of neutron wavelengths reaching the sample, allowing the coverage of several orders of magnitude in length or time on a single instrument.

b) Are there emerging techniques that should be considered for placement at one of the sources?

Work on several new techniques was presented to the committee, including Larmor labeling, spherical neutron polarimetry, dynamical nuclear polarization and Wolter optics. Each of these efforts appears to be well-supported and making significant and steady progress and there will likely be multiple opportunities for deployment at each of the three sources in the future. The IAB encourages on-going evaluation of the integration of these techniques into user instruments depending on the success of current R&D efforts. In the past, it has taken some time for new neutron methods to be adopted by the broader user community and we would expect the same phenomenon to manifest with these new techniques. Success will likely be tied to the demonstration of significant scientific advances that are enabled by the new methods.

**Wolter optics**

The continuous development of advanced neutron optics has been one of the primary avenues of creating ever more capable neutron instrumentation. Wolter optics, a reflective lens, are the most promising new technology that can continue this trend into the future. These lenses, which can focus a polychromatic beam, are made of Ni and work best for cold neutrons possibly providing gains of more than an order of magnitude. These are far beyond the early development stage as NASA has launched these optics into space as part of the Chandra x-ray telescope. While these lenses were deposited on glass substrates, they are now making these optics from free-standing films. In collaboration with other facilities and the MIT effort, the IAB believes that ORNL should consider how to contribute to advancing this technology.

**Detectors**

With the $^{3}$He crisis in the mid-2000s, many neutron facilities accelerated their detector development programs to replace $^{3}$He detectors. To better coordinate these efforts, a large collaboration was initiated among major neutron facilities in 2010. ISIS, SNS, J-PARC and PSI worked to further develop scintillation detectors, while the ILL, ESS and other European facilities participated in B-coated detector development and in refurbishing $BF_3$ detector technology. Even before this, ORNL developed a scintillation detector system that was deployed on POWGEN, VULCAN etc. Unfortunately, there have been some issues with these detectors and VULCAN is replacing theirs with $^{3}$He detectors and POWGEN is moving to newly developed scintillation technology. We trust these new detectors will perform well. Note however, that scintillation detector systems at ISIS and J-PARC have been working well and NIST has just developed new technology for the fabrication of scintillation detectors that enhances their performance. The IAB believes it is important for ORNL to continue to develop scintillation detector systems and to exchange technical information with other neutron facilities.

**Computing**

Computing is becoming increasingly important for handling and analyzing neutron scattering. For example, DFT calculations are routinely done in conjunction with neutron vibrational spectroscopy. Moreover, the volume of data generated by certain ORNL instruments is too large to be treated by researchers using the computing infrastructure at their home institution. ORNL is a center for high performance computing. Therefore, the IAB believes that ORNL should work to further develop synergies between high performance computing and neutron measurements.

**Moderator and reflector**

The detailed cross section of H-molecules only became available in late 1990's. This was too late for the FTS design to benefit from the use of para-hydrogen in the moderator design. J-PARC has since shown the performance advantage of para-hydrogen with a pre-moderator, and now all new $H_2$ moderators are using this technique to enhance performance. The ESS has made additional improvements, developing a low-dimensional moderator system. STS is taking full advantage of this knowledge, experience and technology. While the FTS is not optimized for para-hydrogen moderators, it is worth studying the neutronics performance gain, and perhaps include a para-hydrogen converter in the $H_2$ cryogenic circuit when there is a major replacement of the target and moderator system.

Quite recently, the ESS has discovered that the performance of the Be reflector is very sensitive to the texture and quality of the material. While this is an ongoing development, it may provide an avenue to improve the Be reflector at HFIR.

**Pulse shaping and multiplicity**

Repetition Rate Multiplicity (RRM) was first demonstrated in the 1990's. RRM has now become a normal operational mode of several regularly operating instruments. Since this technique is indispensable for a long pulse neutron source, most of ESS instruments are designed with RRM in mind. Since FTS operates at 60 Hz, the use of RRM there has been limited. However, STS will produce a broad peak with a much lower repetition of 15 Hz. Therefore, the use of RRM can benefit inelastic scattering instruments at the STS. A chopper can be used to sharpen the peaks produced by the STS moderators making an instrument high resolution. The IAB believes that instrument designs for the STS and the decisions of which instruments to move from FTS to STS should also take these considerations into account.

**Nano diamond reflector for beam extraction from moderator**

There is a program coordinated by IAEA that aims to drastically improve available neutron fluxes. One idea being explored is beam extraction using nano-diamonds. This material is very durable even in a high radiation fields and can be placed at a short distance to the source. Recent results are quite promising for cold neutrons. Although this technique is under development and a robust fabrication method must still be realized, it is worth studying the performance of this technique for the STS and HFIR.

c) Have we maintained sufficient flexibility in our plans to allow for future innovation in instruments and methods?

In the context of the three source vision it is not at all clear that the heavy focus on squeezing every single neutron out of the HFIR cold guide hall, even the less than optimal CG4, is the best use of limited resources. Firstly, if further simulations confirm that the long term strength of HFIR is its thermal capabilities, it would seem that limited resources would be better spent focusing on modernizing, prioritizing and innovating the thermal instrumentation suite as recommended in the "2017 Review of the Instrument Suite for Inelastic Scattering" report. Such an optimization should include re-prioritization of instruments, considering removal of instruments that will do significantly better at the FTS or STS, adding new high impact instruments such as a thermal imaging station for example, and fully updating/upgrading the world class thermal triple axis (including the not yet approved upgrades to some of the backends).

The cold neutron guide hall at HFIR is at capacity. The Be-reflector replacement will provide an opportunity to reoptimize the instrument suite. ORNL should take this opportunity to develop a modern cold triple axis – an instrument which will not be superseded by the STS. ORNL should also carefully consider imaging in light of the three source vision with the aim of providing the best instrumentation for the US for this emerging technique. It is also essential that a ORNL develop a plan for NSE that results in an instrument competitive with IN15 at ORNL. Further, a 3rd SANS will only increase the US capacity by about 10-15% and the plan to move it to STS later along with the other two SANS instruments currently at HFIR, fails to address the role of the HFIR cold guide hall in the three source vision and leaves a big gap in its instrument suite.

Making a beamline available at SNS as a test station is an important component for maintaining flexibility. This test station might have a modular design to make reconfiguration easy. A test station will be especially helpful for aiding in the design of instrument concepts that have yet to be built anywhere else, developing proof of principle concepts and technologies for STS. The ORNL team has proposed such an instrument before (INVENT) although it was not discussed and not considered a high priority.

Building new instrumentation in a modular fashion maintains maximum flexibility. However, the IAB feels that a modular approach for easily moving beamlines could be counterproductive as any such move could severely inconvenience the scientific community.

A critical point, and one regularly mentioned but often ignored in practice, is the fact that the productivity of an instrument depends on much more than its performance. The IAB strongly encourages ORNL to take a holistic approach to instrument design rather than simply provide "flexibility" for everything else. This means thinking about sample environment and software development needs (not only data acquisition but reduction and analysis) as an integral part of the instrument planning phase. Maximum productivity of any instrument will only be met when considering all these aspects of an experiment. For example, if a new instrument collects data at a much higher rate than current instruments, sample environments must not become the rate limiting step. If necessary, new technology in sample environment must be realized simultaneously with instrument implementation. Space must also be well thought out to allow for the flexibility of different sample environments required by users. Also, if adequate, user-friendly software is not developed to handle the large amount of data generated by a new instrument, then productivity will not improve. Therefore, it should be a top priority in the development of any new instrument to make a comprehensive plan that includes every aspect of importance to the user.

Finally, it should be emphasized that there is a critical need to maintain space in the budget to allow for integration of future innovations into the proposed new instruments. In this context, the lack of nearly $6 million to complete the proposed instrument buildout with the plan to get partners to make up the slack is a bit worrisome. It is not clear that such partners can be found given the constraints of the facility and an open access beamline. It would be prudent for ORNL to seek ways of developing and funding these instruments completely rather than piecemeal. While some of these funding avenues could involve innovative ways of engaging industry to have a role in instrument development, the facility should think more broadly about alternative funding streams as well as a contingency plan should such funding not be forthcoming.

**II) Priorities for improving existing instruments and building new instruments at FTS and HFIR**

a) Do the current ORNL instrument suites represent a balanced portfolio of capabilities that is expected from a major center for neutron scattering?

b) Are there gaps in capabilities or capacities we have identified that should be addressed with high urgency? Are the priorities identified for near term (0-5 years) investment appropriate?

**Imaging**

Neutron imaging is a powerful technique for the 3D visualization of materials that range from fundamental new systems through to device components; complementary to other techniques, neutron imaging offers unique insights into the materials world and, as such, it is essential that neutron facilities provide this capability. ORNL, with its existing facilities, HFIR and FTS, and the future opportunities afforded by a STS, has the potential to provide a world-leading suite of neutron imaging instrumentation. Currently, CG-1D, the cold neutron imaging instrument at HFIR, is the only imaging facility at ORNL. With limited resources, CG-1D has produced a significant amount of valuable research. The proposal to construct VENUS, a platform for studying materials and engineering components on the FTS, is an important and essential development in establishing ORNL as a world-leading neutron-imaging institution. VENUS should be operational by the time of the HFIR outage so that ORNL maintains a neutron imaging capability throughout this period. Finally, ORNL must develop a plan for imaging taking into account the three source vision. This plan should consider the potential of imaging instrumentation using both thermal and cold neutrons at HFIR and at the STS in addition to VENUS and the cold neutron imaging station at HFIR.

**Diffraction**

Single crystal diffraction covers a very broad range of science from the detailed diffuse scattering of fundamental condensed matter systems through to biological macromolecular crystallography. There is an existing extensive portfolio of single crystal instruments at HFIR and SNS-FTS. Careful consideration, over the next five years, of future opportunities should be undertaken with a view to rationalizing single crystal instrumentation on HFIR, FTS and a future STS to ensure the optimal coverage of the future scientific challenges in neutron single-crystal diffraction.

Powder diffraction is a key technique for the characterization of both fundamental and applied materials systems. The current powder diffraction instrument suite at ORNL produces high quality science but is outperformed in many areas by the instrumentation at ISIS and J-PARC. The near-term construction of DISCOVER and HighResPD is essential to establish ORNL as a world leader in neutron powder diffraction (NPD). DISCOVER builds on the existing excellence at ORNL in NPD and, in particular, PDF analysis, and will result in world-leading capabilities in combined NPD and PDF. HighResPD will provide high flux and very high resolution that is comparable with synchrotron X-ray powder diffractometers. HighResPD is necessary for the complementary analysis of X-ray and neutron powder diffraction measurements of structural complexity ranging from subtle structural phase transitions in fundamental materials to microstructural imperfections associated with real world issues such as catalysis, battery cycling and materials degradation. The recent decision to move HighResPD from an STS instrument concept to a shorter-term project for FTS makes sense for several reasons. First, it will bring this much needed capability online sooner. Second, HighResPD can be implemented at FTS with little performance impact and is consistent with the three source vision. It also allows the STS design to be fully optimized for cold, low- to medium-resolution applications, without compromise. In preparation for a future STS, it is important to consider, in the near future, the opportunities afforded by a medium resolution, cold- neutron powder diffraction (WISH-type) and a medium resolution combined high Q and small-angle total scattering instruments (SWANS).

**Spectroscopy**

FTS and HFIR have extensive capabilities in neutron spectroscopy for quantum materials, chemistry, and catalysis. The clear capability gap in this suite is cold-neutron triple-axis spectroscopy, which most directly affects quantum materials research. While the CTAX instrument fits this profile, the low flux and lack of polarized beam capability limit its scientific impact. A competitive cold triple-axis spectrometer is needed at HFIR to complement the highly productive CNCS instrument at the FTS. The MANTA instrument concept is currently being developed and has strong community support. ORNL must strongly pursue simulations of MANTA to confirm its performance as world-class instrument.

Investment in MANTA, and the cold source in general, must be balanced with the urgent need to modernize thermal triple-axis capabilities. These instruments have not been updated in decades. Newer concepts in thermal triple-axis spectrometers (such as a multianalyzer backend) have been employed at other facilities with great success. Here it seems that the opportunity and indeed the necessity of reoptimizing the cold guide hall during the outage for the Be reflector conflict with the long-term three-source vision which places emphasis on HFIR's capabilities as a premier thermal neutron source. ORNL should think carefully about this tension and come up with a plan that also ensures the long-term sustainability of the HFIR thermal instrument suite. As an example of a particular trade-off, the IAB notes that most of the improvement on MANTA will come from the improved guide system. We therefore believe that ORNL should operate MANTA with the current CTAX secondary spectrometer.

The HIGGS inverse geometry spectrometer was proposed as new instrument concepts for FTS. As HIGGS covers similar science as the thermal direct geometry spectrometers, there is not an urgent need. However, the concept should be explored as it promises to deliver much higher counting rate, albeit with reduced flexibility and the potential for much higher background. This is a concept that can be more straightforwardly employed with cold neutrons and should be explored for STS.

BeFAST is another proposed inverse geometry spectrometer that would be a low-resolution version of VISION. It would extend capabilities for chemical spectroscopy, but is not an urgent short-term need.

**Neutron Spin Echo**

Traditional energy-resolving neutron spin echo (NSE) is critical for soft matter researchers, as it provides unique sensitivity to very slow motions inaccessible by other techniques (neutron or otherwise). Unfortunately, the NSE situation in the US is far from satisfactory. Currently the US scientific community lacks access to an instrument capable of measuring the same time-range as IN15 at the ILL placing them at a significant disadvantage. The single NSE instrument at ORNL is not globally competitive and there is little the SNS can do about this until they are able to take full responsibility for the instrument in 2020. Per the 2017 inelastic suite review, BL-15 at SNS is limited to a maximum Fourier time of 150 ns. The only other NSE in North America (at NIST) can measure out to 300 ns, while IN15 at ILL regularly measures out to 600 ns. In principle, a new NSE competitive with IN15 could be constructed at an end guide position viewing the HFIR cold source although it is possible that the STS would be the best long-term source. ORNL proposed to attempt to double the maximum Fourier time of the existing NSE through the installation of new compensation coils sometime after 2020. The IAB believes that this approach is inadequate, rather it is essential that ORNL produce a long-term approach to developing a truly forefront NSE instrument in the US. The IAB understands that this will take a major effort requiring significant contributions from international experts. A final plan needs to be based on a detailed technical evaluation that includes a complete understanding of the reasons for the disappointing performance of the NSE at the FTS. Given significant current need and the long lead time for developing such an instrument, it is imperative that ORNL begin the process immediately.

**SANS**

The ORNL SANS suite features 3 SANS instruments plus a USANS instrument. All are oversubscribed, and the proposed addition of a new SANS in the HFIR cold guide hall would certainly be well utilized by the US scientific community. However, there are already 9 SANS instruments, including 7 pinhole machines in the US providing a wide range of capabilities. Therefore, the additional capacity provided by an 8th pinhole SANS instrument is not very compelling. In addition, the idea to build a new SANS in the HFIR cold guide hall, and then move it to the second target station (STS) would cost significant resources and disrupt the SANS user program. Given that there are critical gaps that the facility should address, and that SANS instruments are expected to perform very well at STS, it is sensible to avoid moving instruments to the extent possible, and plan for one and probably two SANS specifically designed for placement in the STS. The IAB believes that the planned move of USANS to HFIR should be pursued. It will improve performance while freeing up needed real estate at FTS.

**Reflectometry**

ORNL currently operates two world-class reflectometers at FTS. Capabilities exist for liquid samples, vertical geometry, polarization, and polarization analysis. A third reflectometer for the HFIR cold guide hall was proposed as a low priority. We agree that this is a low priority and instead recommend focusing on reflectometry at the STS, where truly game-changing instruments can be constructed.

c) Are we effectively identifying and realizing new opportunities in neutron sciences that could be optimally addressed at FTS or HFIR?

One clear gap in US capabilities which has been pointed out by several panels and committees, including the "2017 Review of the Instrument Suite for SANS/Reflectometry..." is the low q, long time scale dynamics that an IN15 class spin echo machine would provide. This is particularly important for the soft matter community. Combining structure with dynamics is emerging as the next challenge akin to the multiscale challenge of the past decade that SNS and HFIR have been working to address in all their new instrumentation. There is currently no such capability in the US and the HFIR cold source is currently the only place such an instrument could be built, thus presenting a unique opportunity. While the IAB appreciates the risks may be quite high given the expertise of the lab and complexity of the instrument, we strongly recommend that this option be considered more carefully and that a plan be developed immediately that will result in an NSE instrument that is competitive with IN15.

The closure of two major neutron sources in North America (the Lujan Center at LANSCE in New Mexico and Chalk River National Laboratory in Canada) has resulted in a crisis for the scattering community. The Lujan Center, for example, was a mecca for nPDF (neutron PDF) analysis of disordered materials. ORNL is proposing to build DISCOVER - which will fill a need for nPDF in North America. Much of the Lujan talent has already relocated to ORNL and there is an opportunity for ORNL taking a real leadership role in this area which they should fully embrace. Similarly, Chalk River was a center for applied neutron diffraction through the ANDI program (Applied Neutron Diffraction for Industry). This is another opportunity to build upon this expertise with applied neutron diffraction on instruments such as VENUS (building on the success of instruments such as VULCAN).

d) Are we missing critical areas for further scientific and technical innovation?

Studies of heterogeneous materials, especially soft matter and glasses, have begun to show that imaging correlations in real-space and time through the correlation function G(r,t) can sometimes provide scientific insights not available by looking at S(Q,E). This method often requires that data from various spectrometers, each covering different Q and E ranges with different resolutions, to be combined and Fourier transformed. The procedure requires careful statistical treatment using, for example, maximum entropy methods and has not yet been widely adopted. Opportunities may also be available to measure G(r,t) directly using Larmor labeling techniques over suitable ranges of r and t. These areas may be an opportunity for ORNL to take a lead in view of the wide dynamic ranges of its spectrometers, their institutional excellence in computing and their emerging expertise in Larmor labeling methods.

The need to access a wide range of parameter space is becoming increasingly important, as the systems under study become more complex and more in-situ and in-operando measurements are performed. This will benefit from the construction of instrumentation where neutron methods are combined, such as: spectrometers with diffraction capabilities which allows following dynamics and excitations through a well characterized phase diagram; diffraction instruments that probe a wider range in Q-space realized as a SANS instrument designed with a medium angle detector or a diffractometer with a SANS detector (SWAN proposal); and/or wide energy coverage in reciprocal space via combining direct and indirect spectroscopy methods.

The high brightness of SNS and HFIR sources provide opportunities to observe phenomena in a real time (kinetics) and to perform faster measurements (high-throughput), but these experiments must be enabled by appropriate resources. To this end, automation should be seriously explored for sample loading and changing, as well as remote handling and software for data reduction and analysis. Similarly,

in-situ and in-operando measurements are in high demand (e.g. catalysis or conventional chemical reactions, recent experiments on VULCAN on an operating engine, polymer processing), enable new and exciting science and discoveries, and attract interest from industrial stakeholders. Careful consideration of the implications on the instrument scientist and sample environment teams in terms of design and operation of new equipment, as well as time and staff effort is imperative. Furthermore, an engagement with the existing user community and outreach into new ones are key to identify demands alongside a strategic deployment.

An easily reconfigurable test beam port has an important role for various development purposes, including detectors, optical components, methods development etc. Beam ports that lack sufficient space for a full-scale neutron instrument would be a reasonable place for a test station such as INVENT. Although there is a test port at HFIR, pulsed neutrons provide unique capabilities that make such a port essential, particularly considering the need to develop ideas for the STS. We thus encourage SNS to make such a port available.

Consideration should be made of the use of the epithermal neutron spectrum available at SNS for testing single event effects and more generally for neutron irradiation. A beamline dedicated to this, similar to the ChipIr instrument at ISIS TS2 would provide a unique capability to the US community.

Since SNS is funded by the Basic Energy Sciences division of DOE, industrial use of the facility has not been aggressively pursued. However, neutrons are becoming increasingly important to industry. J-PARC is a good example, where more than 30% of experimental proposals come directly from companies. There are also new efforts in Europe, to encourage industrial use of neutron and photon facilities. It is worth looking at a recent Focus feature in the October 2017 issue of Physics World magazine, on "How industry exploits neutrons". Often industry is unaware of how neutrons can help their companies and thus, suitable outreach efforts are required to stimulate them to use neutrons.

**Thanks**

The IAB thanks ORNL for the hospitality and their openness in presenting their ideas. We also appreciate that ample time was provided for discussion in executive session. It certainly made our job easier.