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HEIMDAL Optics design

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This report describes the guide system for the thermal powder diffraction part of the instrument HEIMDAL along with the first 28 m of cold guide for the SANS option. The thermal part of the instrument should be able to run in four different resolution modes, ranging from high resolution mode (σd/d=0.1%) to high flux mode (σd/d=0.7%). The instrument resolution is tuned by changing the incoming divergence on the sample using a slit system in the last part of the thermal guide.

A presentation of different installation options for the cold guide in the guide hall (E02) can be found in the report “Cold guide options, Instrument : HEIMDAL”.

General considerations

The beam requirements for the HEIMDAL diffractometer and SANS upgrade are very different. SANS requires cold neutrons with divergences of up to 0.1° and prefers energy resolutions of ~10% while the diffractometer is designed to have access to thermal neutrons with 0.1° to 0.5° divergence and 1% to 0.05% energy resolution. While a bi-spectral extraction could mix cold and thermal neutrons it would not solve the issues of different resolution requirements. Furthermore, the direct thermal beam would harm the SANS detector. Instead a two guide solution is envisioned.

The guide designs are almost independent and will be treated in two different sub-chapters as the thermal diffraction guide have the hardest requirements it will take priority whenever there is a discrepancy between their priorities.

Thermal Guide

Instrument requirements

The neutron optics system has been optimized for the transport of a typical beam collimation of +/-0.5° (horizontal and vertical) on a 0.5 cm wide and 2 cm tall sample. The collimation can be controlled by using divergence jaws, a slit system known from WISH, ISIS. Finer collimation is advantageous when a fine σd/d resolution is required, while a narrower collimation enables to match the coarse time resolution of the high flux modes. The thermal neutrons optic system is optimized for a fixed wavelength frame of 0.5 Å – 2.2 Å.

The integration of the choppers has been taken into account from the principle. Especially the integration of the Pulse Shaping Chopper (PSC) implied to constrain the horizontal dimensions of the guide at the exit of the insert placed inside the monolith, which is now fixed to 30 mm. The pinhole will also be key in limiting background and shielding cost so a 100 mm gap should be left for a tungsten background collimator in front of the PSC.

In the current model does not included gaps for the integration of Prompt Pulse Suppression (T0 choppers), which are 335 mm, leaving space for a T0 chopper as proposed for DREAM as a way to block the prompt pulse [ref ESS Neutron Optics Group study from June '15]. The losses due to the gaps are estimated in around the 12% of Brilliance Transfer. This value is estimated comparing guide layouts with and without gaps. The losses can be significantly reduced when a guide element is inserted in the 20 cm gap in between the two hammers. A technical solution has to be worked out in which the guide element is integrated in the chopper housing.

Spatial Constraints

The HEIMDAL pilling corridor in the E02 hall is shifted 1.3 degrees compared to the W8 Beam Port Coordinate system used for the monolith and bunker sections of HEIMDAL. This imposes severe constraints on the shape and orientation of the guide, forcing it to have a fairly narrow feeder, looking at the northern end of the thermal moderator and blocking the entire monolith at the moderator height. Furthermore, the thermal guide is required to travel along the edge of the piling corridor because of the above constraints (See figure 1).

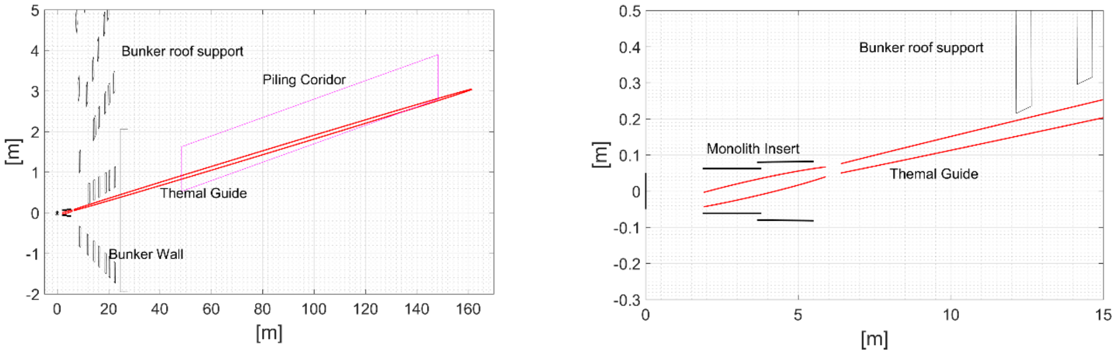


Figure 1: Spatial constraints for the thermal guide. The pilling corridor is shifted 1.3 degrees compared to the ISCS, placing heavy constraints on the position of the guide.

The guide can start 2 m from the target coordinate system (TCS), or 1.89 m from the W8 Instrument coordinate system (ISCS). The Light shutter ends 5.98 m from the TCS or 5.87 m from the W8 ISCS. An extra space of 420 mm is required before the pulse shaping choppers to enable choppers + rotors to be lifted. Thus the pinhole between feeder and main guide will be located 6.29 m from the W8 ISCS. The T0 chopper and heavy shutter need to be located inside the bunker, *i.e.* no more than 24.03 m from the W8 ISCS, with the later preferably placed next to the bunker wall. The guide should end at 158 m to provide space enough for the instrument cave and sample environments.

Optimization of Guide

The guide optimization was performed using the neutron Monte Carlo raytracing package McStas and the guide_bot tool for McStas. To avoid the optimization algorithm settling in suboptimal local maxima all optimizations were run at least 6 times parallel and compared. Whenever the comparison suggested that that the algorithm had difficulties reaching an acceptable maximum the number of optimizations was increased until a satisfactory maximum was reached. Furthermore, as the possible parameter space is immense the optimization was performed in a number of steps. For each step the 2-3 best performing optimizations were kept and investigated in parallel with 6 new optimizations in the next step.

A general study of guide geometries and pinholes were performed. To achieve an overview of principal guide geometries a large study was performed for HEIMDAL and BIFROST. The investigated guides were: A simple long ellipse, Two Ellipses separated by a pinhole, 3 ellipses separated by two pinholes, three ellipses separated by a pinhole and a kink to get out of line of sight, and a double bender. Each geometry was optimized for a number of different wavelength bands. For the pinholes both length, width and height were investigated and a pinhole size of 30 x 50 mm^2 was found to be optimal, while pinhole lengths of up to 50 cm was found acceptable. With these sizes fixed the guides were optimized for both price and performance, using neutrons per Euro as metric. The study will be described in further detail in the report Optimizations of the long neutron guides for the ESS instruments HEIMDAL and BIFROST and gives a strong backbone for further optimizations.

A number of guides was studies in less detail. To expand the investigated geometry space a number of guides were studied in fewer settings than the guides in the backbone study and compared to the backbone guides. Previous studies have shown that kinked guides can perform better if short straight sections are inserted before and after the kink. Recent studies at PSI have however suggested that this is only true if LoS can be lost very far from the source and the optimization confirmed this. Even here the gain was minimal.

A solution where an absorbing rod was placed in the middle of an ellipse in order to block LoS was investigated. The resulting brilliance transfer was low and the phase space undesirable. To improve performance a reflecting nose was placed in front of the rod, reflecting desirable neutrons away from the beam stop, the beam stop was covered in neutron mirrors, and a second nose placed after the beam stop to connect the phase (see Figure 1). By optimizing the shape of the noses it was possible to improve the solution however it never became competitive at short wavelengths and was thus discarded for HEIMDAL.

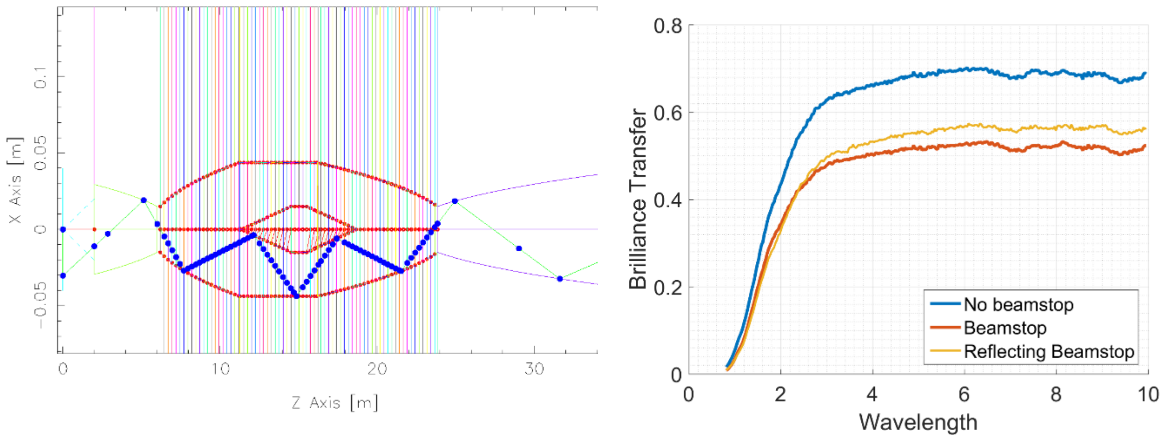


Figure 1: Simulations of a reflecting beam stop inside the guide to block LoS. Left: McStas model seen from above. Right: Comparison of brilliance transfer for a guide without beam stop, a guide with beam stop, and a guide with optimized reflection noses at the beam stop.

The kinked section was replaced by a curved section in the kinked backbone guide. This provided the most promising result for guides loosing LoS and was optimized for several different LoS settings.

A guide solution was chosen. Combining the results from above with result from the DREAM study of fast neutron background the elliptic feeder and single ellipse guide with a 30 x 50 mm^2 pinhole was chosen as it had the best Brilliance transfer, smoothest divergence profile and lowest price. The background suppression is slightly worse however the instrument will be utilizing a T0 chopper in all setting reducing the fast neutron background at sample position to an estimated 750 n/s of which most will not interact with the sample. The resulting background will be many orders of magnitude below the incoherent background from a sample illuminated by ~10^9 n/s. In order to ensure that this solution was not outperformed when specifications changed, a curved guide was optimized for reference whenever changes was implemented in the guide geometry.

The geometry was tested against the geometrical constraints. In particular, the shifted axes of the piling corridor posed a challenge for the straight beam path, however since the width of the feeder have a very limited impact on guide performance a modification with a narrower feeder was chosen.

A study of different wavelength bands was performed. In order to ensure that HEIMDAL does not sacrifice to much traditional diffraction performance by optimizing for 0.5 Å neutrons required for PDF analysis several different wavelength bands were studied: 0.5 – 2.2 Å as the preferred band, allowing full PDF analysis. 0.6 – 2.3 Å to study how a limited PDF would impact the performance of HEIMDAL, and 0.8 - 2.5 Å to investigate the performance of a non PDF solution. In all solutions PDF can be omitted by changing chopper phases, however if a guide optimized for 0.8-2.5 Å would show considerably better transport capabilities the choice of PDF could be reconsidered. Simulations showed a limited performance increase for such guides, proving that the scope of the instrument should not be decreased.

The shape of the guide was re-optimized with a finer model. The guide shape was re-optimized including more detail for choppers and geometrical constraints. This was at first performed using m=6 mirrors.

The coating was optimized taking cost into account. Coating_writer, a plugin in guide_bot was used to optimize the coating throughout the guide. To keep the number of free parameters at a realistic value the guide geometry was frozen, however the optimization was performed for several high performing geometries to counter the risk of moving towards a local maximum.

Bi-spectral option was tested. In order to increase the flexibility of the diffractometer a bi-spectral upgrade was investigated. Simulations showed that the sides of the monolith insert have no impact on the performance of the thermal guide. The southern side will thus be omitted to allow neutrons from the cold moderator to enter the guide. The monolith plug does however shadow the cold moderator, limiting the amount of cold neutrons that will reach the possible bi-spectral switch position. The northern side have thus been re-optimized to reflect cold neutrons into the light shutter (see Figure 2). Currently the extra cold neutrons will not reach the sample. It has however been simulated that a later Bi-spectral switch upgrade in the light shutter will improve cold neutron performance in this setup. This switch has not yet been optimized and will be a future upgrade path.

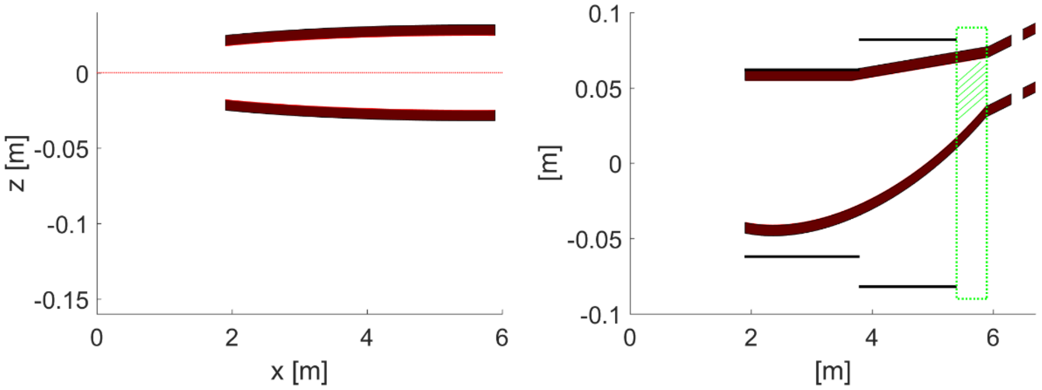


Figure 2: The monolith insert. Left: seen from the side. Right: seen from above. The blue Is the cold guide, the red the thermal guide, and the green the light shutter and possible bi-spectral switch upgrade.

Layout of the guide

The vertical and the horizontal profiles of the guide are shown in Figure 3. The guide is currently an elliptic feeder plus a long elliptic guide. The long elliptic part will be replaced with a straight guide with elliptic extremities in order to save cost and ease maintenance of the guide. This have been shown to be achievable with almost no loss of brilliance transfer at for example BIFROST. A zoom on the monolith insert can be seen in Figure 2.

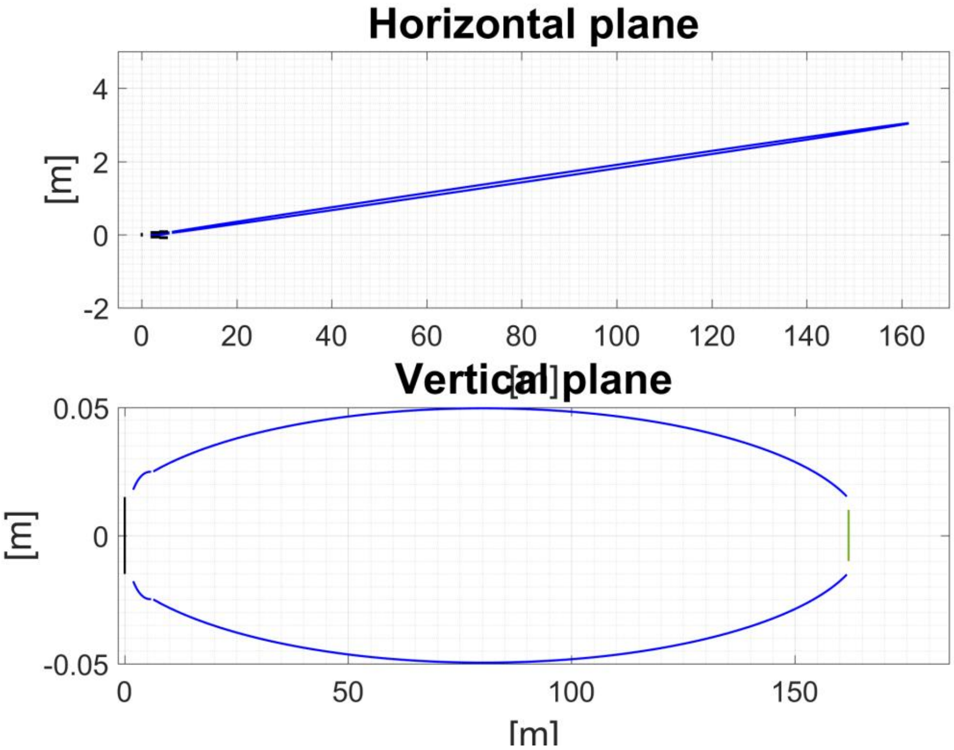


Figure 3: Schematic of the HEIMDAL thermal guide.

Guide Performance

The brilliance transfer and flux on sample can be seen in Figure 4 while Figure 5 displays the beam and divergence profiles. The numbers are given for the guide with all choppers and slits fully open. Flux numbers on sample with choppers running and divergence jaws in use will be between 3 and 10^3 times lower depending on the desired resolution. The estimated guide price is 2.2 MEuro.

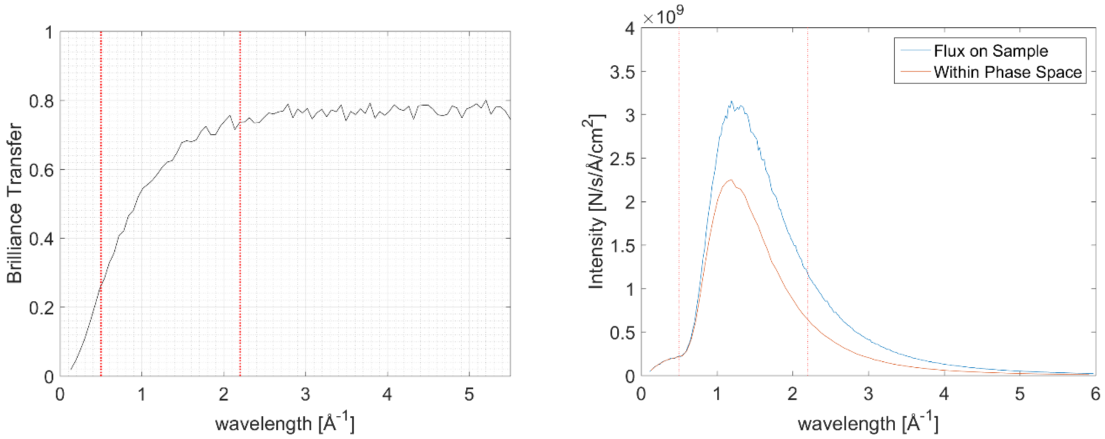
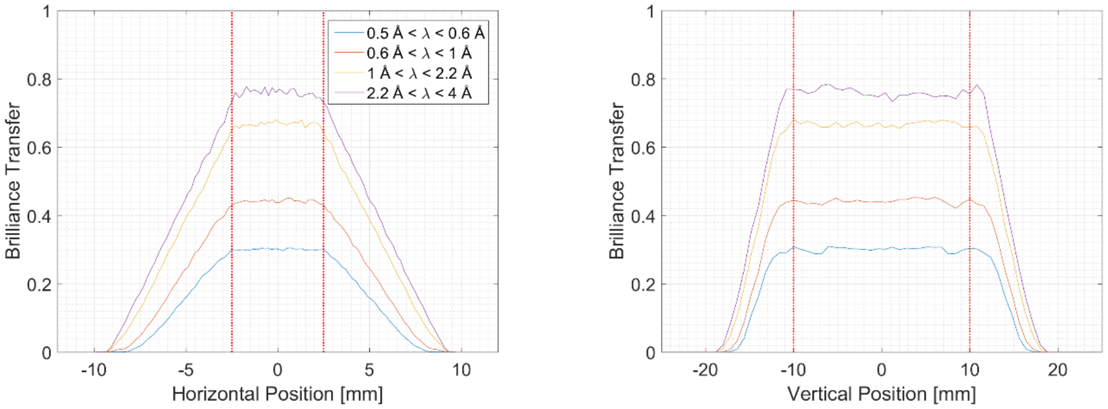


Figure 4: Brilliance transfer (left) and flux on sample (right) for the thermal guide.



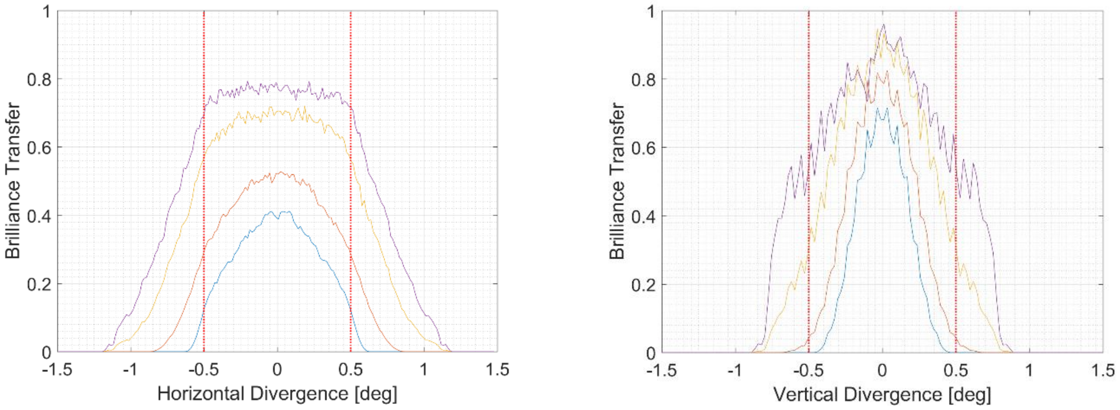


Figure 5: Beam and divergence profiles for thermal guide.

Cold Guide

Only the cold guide inside the bunker will be part of the instrument construction project. The rest of the guide is however also considered to ensure that the first 28 m will provide a useful beam for the remaining guide.

Instrument requirements

The guide is required to transport neutrons to the collimating section starting 11 m before the sample. Here a beam diameter of 16 mm and a divergence of +- 6 arch minutes are required. Wavelengths above 4 Å should be transported.

The guide will have 3 choppers. 2 frame overlap choppers at 12 and 14 m and a band selection chopper at 80 m.

Spatial constraints

Thermal guide has the priority when the two guides have conflicting interests. The choppers of the two guides cannot intersect the other guide are required to have a simple extraction system for maintenance purposes. Only one set of choppers can have their rotors located on the side of the guides as placing rotors south of the guides would interfere with the T-Rex beamline. It is thus required to have one beamline below the chopper housing of the other beamline (See Figure 6). Furthermore, the thermal guide is blocking the monolith at the moderator height. The cold guide will thus be extracted below the moderator height, this limits the height to 2 cm, which is sufficient to collect the desired phase space. The maximal tilt with full view of the moderator is 1.3°.

The guide is required to achieve a horizontal distance to the thermal guide of 120 mm (center to center) before 6.5 m to pass below the thermal choppers (see Figure 6). The cold choppers will be placed at 12 and 14 m requiring a horizontal distance between the guides of 150 mm to ensure space for chopper housings. After the cold choppers the cold guide should approach the thermal guide to save money by combining both into a single vacuum housing this is achieved by gluing the cold guide beneath the thermal guide before mounting the thermal guide. This requires the cold guide to be situated at a vertical distance of 90 mm once it has passed below all thermal choppers.

At the sample position the beam should be in the horizontal plane of the sample and intersect the thermal beam at an angle of 4.5 degrees.

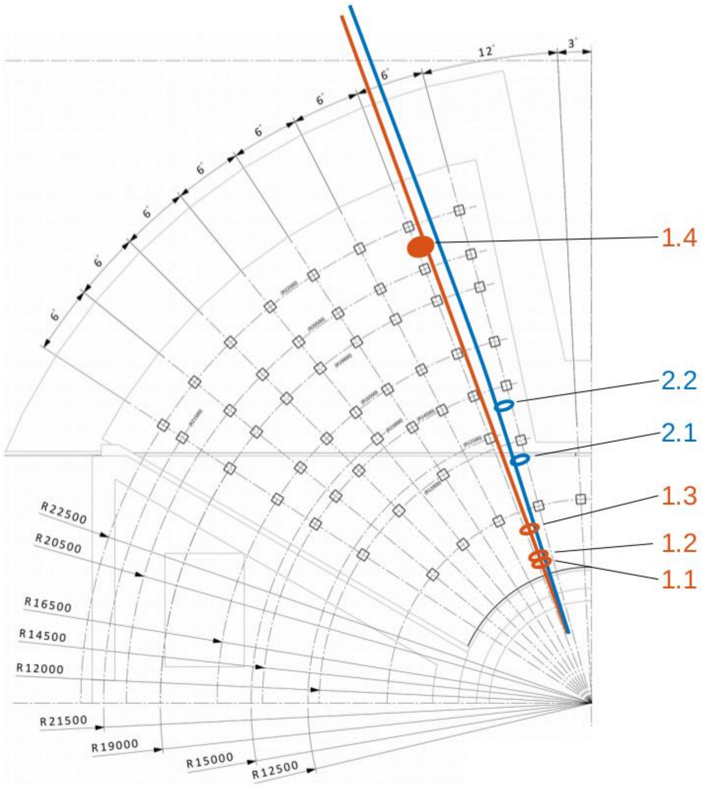


Figure 6: Chopper placement in the bunker. The blue is the cold guide and the red the thermal guide. By placing the cold guide below the thermal guide it is possible to extract all thermal choppers for maintenance. In order to access the cold choppers the cold guide is required to have a substantially different viewing angle on the moderator than the thermal guide.

Layout of the guide

The layout of the cold guide can be seen in Figure 8. The cold guide will start below the moderator plane and point 1.3^{o} down (see Figure 7). In the horizontal plane it will have an angle of -1^{o} to the beam port coordinate system. After 6.5 m it will have reached -148 mm – sufficient to pass below the thermal guide and will bend to become horizontal. After 9 m the guide bends to run parallel to the thermal guide. The two cold choppers are inserted in a short straight section before the guide is bend toward the thermal guide. After the T0 chopper the guide is raised to be connected below the thermal guide. It runs below the thermal guide for 93 m before bending to the south and curving up to thermal beam height. Finally, it is bend back towards the thermal guide.

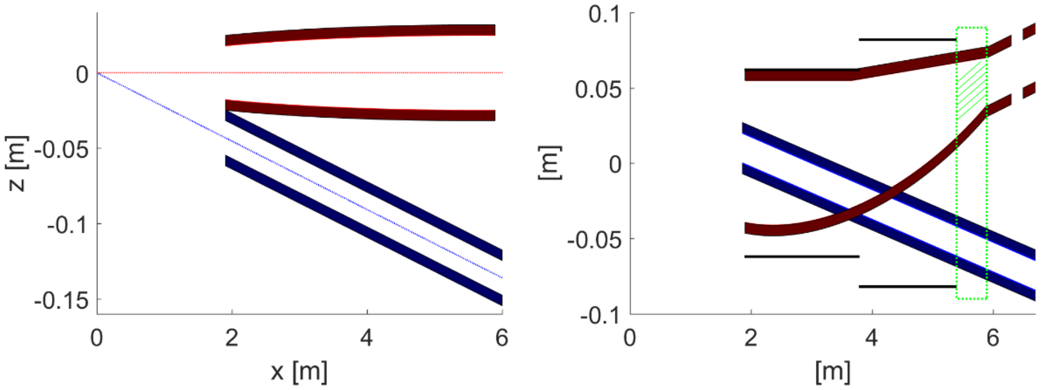


Figure 7: The cold guide in the monolith insert. Left: seen from the side the cold guide (blue) is located just below the thermal guide (red). Right: seen from above the two guides crosses each other. The black shows the boundaries of the monolith and substrates are to scale.

The guide enters the collimating section 11 m before the sample. In order to reach an incident angle of 4.5 degrees while staying on the piling corridor the guide will bend with the use of a single m=5 mirror inside the collimating section rather than a curved section before the collimating section. From a theoretical calculation a radius of curvature of 99 m is enough to transport neutrons above 4 Å if m=3 is chosen in the curving sections. Even if a curvature with this radius will dampen neutrons in the 4-6 Å range due to the lower reflectivity at high q-values, the brilliance transfer will still be acceptable. However, the guide in question contains 10 curved sections so even a dampening of 10% per curve will cause a 65% loss during the entire guide. In order to mitigate this only the first curves where space is limited are designed for 4 Å neutrons. The curves in the remainder guide are designed for 2 Å neutrons instead.

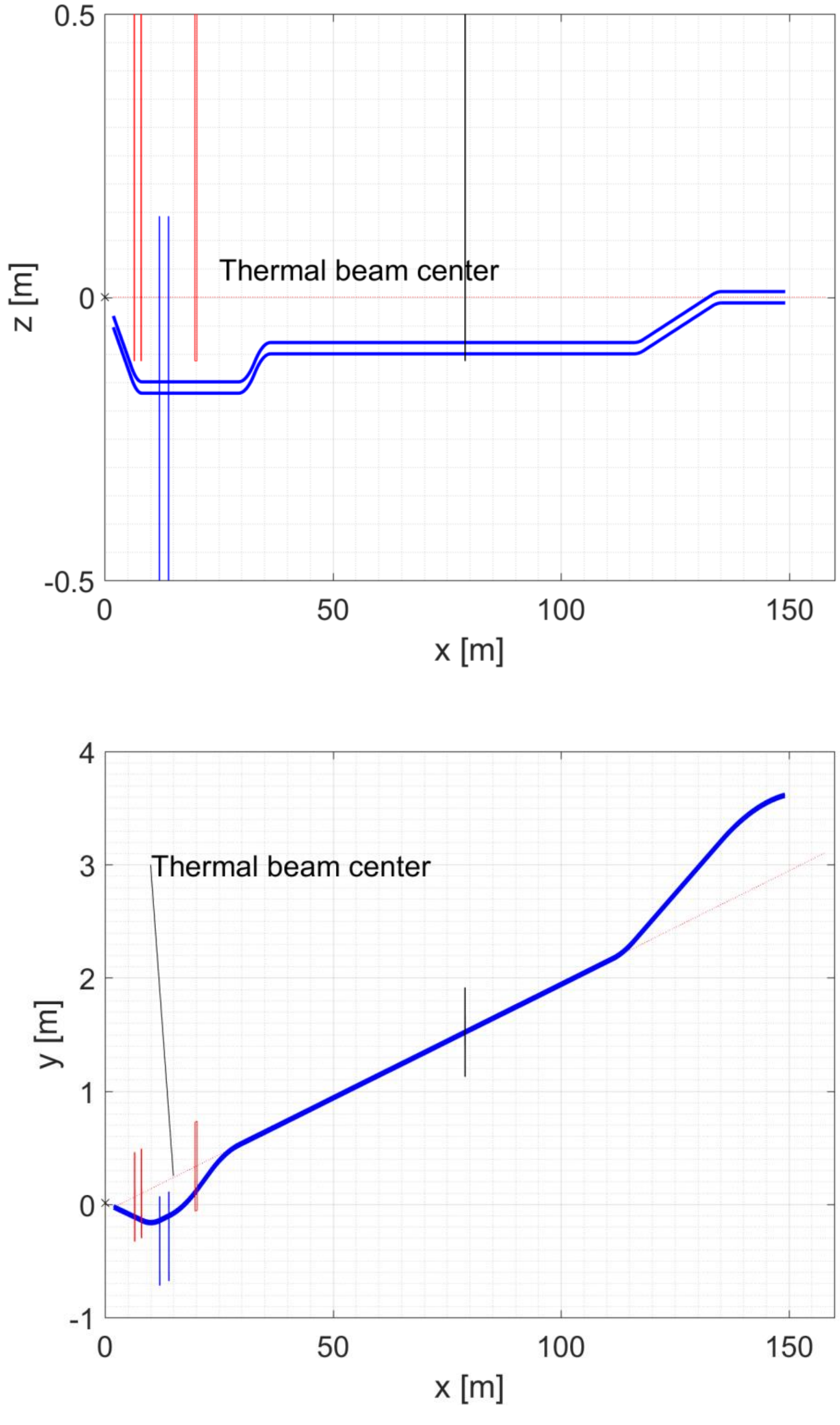


Figure 8: Overall layout of the could guide seen from the side (top) and top (bottom). Chopper houses in the thermal guide are marked with red boxes, chopper houses in the cold guide with blue boxes and common choppers with black boxes.

Guide Performance

The simulated performance of the cold guide can be seen in figure 9. For the coarsest collimation of two 16 mm pinholes 10 m apart. The simulated flux is sufficient to deliver the required performance of the instrument.

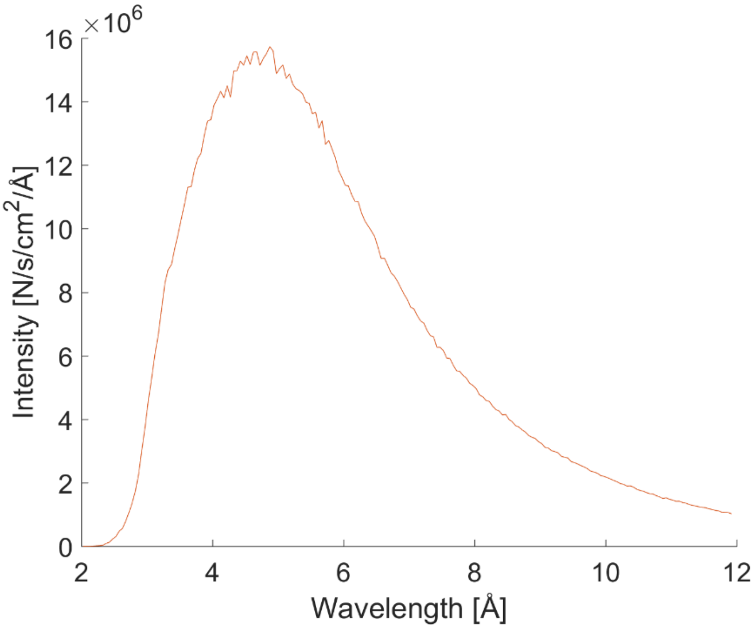


Figure 9: Flux on sample within the desired phase space.

Guide Robustness

A 2x2 cm^2 cross section guide will be relatively sensitive to misalignment problems, however the desired phase space is somewhat forgiving. Misalignments can be dived into two separate effects:

- Translations of guides, i.e. shift between two neighbor guide segments. Swiss Neutronics produces 2 m long guide pieces and quote a tolerance of 2σ = 10 microns at the time of installation (see figure 10 A). This corresponds to an expected loss of 2.5*10^{-2} % of the transported phase space per direction per 2 m, corresponding to a loss of 4% during the entire guide.

- Rotation of guides, i.e. shift between two ends of a single guide segment. Swiss Neutronics reports a tolerance of 2σ = 50 microns the time of installation (see figure 10 B). This corresponds to a standard deviation of 7.2*10^{-4} degrees or an effective decrease of the m-value of 2*10^{-3} for the shortest wavelength of interest in the cold guide.

At the time of installation misalignment of the guide will thus not cause any concerns. It is however likely, that deformations of the ground and vibrations will misalign the guide further during the guide lifespan. Vibrations might cause translations of guide elements thus diluting the phase space. The guides are constructed so they can be realigned from outside to a level of 2σ = 50 microns, corresponding to a loss of 38% for the entire length of the guide assuming all pieces are misaligned. While this is a considerable impact is the very worst case scenario and even this is acceptable from an instrument performance consideration as SANS is a much faster technique than diffraction. Deformations of the ground will furthermore lead to rotations of guide segments. At the intersections between floor sections this can lead to a local shift of up to 3 mm (see figure 10 C). The guide support will translate this into a guide rotation of up to 0.1° for a single 2m guide segment spanning the two plates. This can be mitigated by increasing the m-value close to the floor plate boundaries by 0.2 at 4 Å. It might also be worth mounting several guide elements on a single support beam without pillars connecting them to the ground close to the floor borders (see figure 10 D). This will effectively increase the segment length and thus decrease the possible angle of deflection. While the latter is probably more relevant for thermal than cold guides This should be investigated further in the detailed design phase.

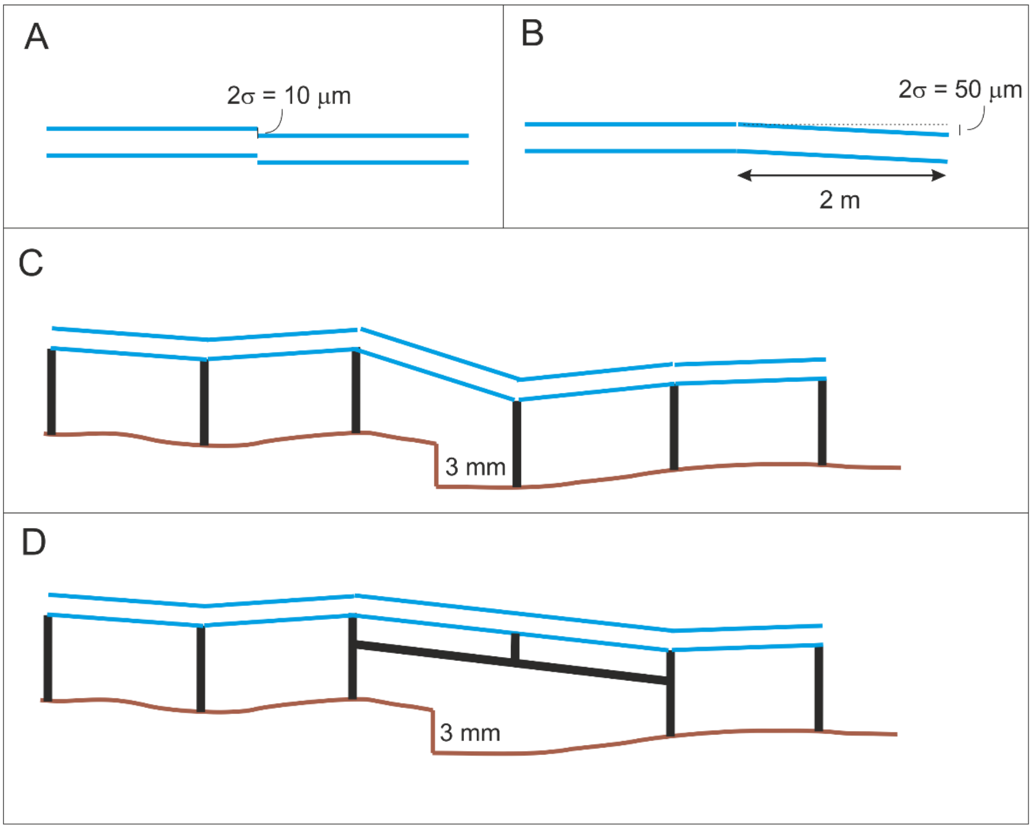


Figure 10: A: A misalignment between two adjacent guide pieces translates into a translation of guide pieces with respect to each other. B: A misalignment of two ends of one guide piece translates into a rotation of the guide piece in question. C: Ground deformations will lead to rotations of guide pieces when the guides share a common mounting at the ends. D: If specific positions are prone to unacceptable high ground deformations (e.g. the boundary between different floor pieces) this can be mitigated by mounting several guide pieces on a single support beam.