Proposal Sample Environments for LoKi

1. **Outline**

As a SANS instrument with a broad simultaneous q-range and high flux, LoKI is expected to cover a wide-range of scientific interests. Therefore, we should firstly look towards the most generic sample environments that will definitely be required at LoKI (and SKADI). Our second consideration should be how best to exploit the high performance of the instrument. With high flux and wide simultaneous q-range, LoKI is ideally suited to studying dynamic systems, which change their structure in both solution and the solid state over short periods of time. Such changes may be induced by internal and external influences, such as flow, stress/strain, temperature, chemical composition, pressure, humidity, magnetic & electric fields. The third consideration is the ever-growing demand and interest in performing in situ and/or simultaneous characterisation of the system under investigation with SANS (and SAXS). The fourth and final consideration is the automation of sample changes. This concept probably needs the most thought/creativity as it is currently the least considered sample environment aspect at neutron facilities.

2. **Sample types**

Sample sizes will typically be less than 10 x 10 mm and may go down to 2 x 2 mm (or smaller). Some typical samples are listed below, but this is by no means comprehensive.

i. Dilute solutions of nanoparticulate materials typically in aqueous or organic solvents
ii. Viscous solutions or gels
iii. Suspended 'solid' materials in solution, such as crushed plant/animal tissue or fuel cell membranes
iv. Solid samples, e.g. rocks, metals, shells, polymers

3. **Sample Environment Equipment Summary**

The proposed sample environments for LoKI given below, fall into four categories depending on their urgency, scientific impact and frequency of use: *essential*, *highly desirable*, *desirable* or *potentially interesting*. Below this list is a general assessment of all the considered sample environments, ranked from 1-5 depending on their perceived priority (1 = low; 3 = essential for day two; 5 = essential for day one). For each case we have justified their need by their *scientific case*, what each needs to be able to do (*required specification*), what it needs in terms of sample environment supplies (*required services*) and integration (*required integration*).

Essential:
- Thermostated sample changer
- Rotating/tumbler cell holders
- Quartz cells of various dimensions

Highly Desirable:
- Rheometer
- Pumps (HPLC and syringe pumps)
- Dismountable 'sandwich'-style cells
- Stopped-flow cell with HPLC pump
- Goniometer

Desirable:
- 1,2-plane shear cell
- Humidity cell / chamber
- High pressure cell

- 3 or 7 Tesla cryomagnet
- Baths/coolers for transport of samples from labs to the sample environment.
- Linkam temperature stage
- Stress/stretching rig for soft matter
- Sample changer with individual/isolated heating elements
- Furnace
- Cryostat

Potentially interesting:
- Ultrasound transducers
- Dielectric and magnetic rheometry
- Sample changer robot
- Couette shear cell
- Smart irradiation set-ups
- 1 Tesla electromagnet with high frequency
- Support for *in operando* battery and fuel cell measurements

Ancillary equipment and facilities:
(some specific equipment that will support the user programme in addition to the general chemistry & biology facilities for sample preparation)
- Transport for heated/cooled samples directly from lab to sample environment
- Dynamic light scattering
- UV/Vis absorption spectrometer
- Glove box
- SAXS
- Centrifuges
- Facilities for cleaning solid samples using Piranha solution

4. SEE Scientific Case and Specification

In order to fully exploit the maximum scattering angle detectable at LoKI, all sample environments should where possible allow scattering angles of up to **45°** with apertures of at least 5 x 5 mm^2. Sample environments should be designed so that they have a constant detector offset every time they are installed. It is assumed that almost all the environments listed below will need access to power and the network and therefore these supplies have not been stated explicitly. The lengths of sample environments given below refer to their length in the neutron beam.

i. Sample changer with (continuous) temperature (priority = 5)

Scientific case	Dilute samples in deuterated solvents loaded into quartz cuvettes are going to be the most frequent on LoKI. Therefore, thermostated holders which can hold a large amount and variety of quartz cuvettes is crucial. Soft matter materials in aqueous and organic solvents (e.g. proteins, surfactants, polymers, suspended nanoparticles) are generally measured between 4-80 (or 150 °C. Solid samples (e.g. metallic samples, rocks, cement) and dismountable sandwich cells for holding materials not suitable for cuvettes (e.g. gels, films, nano-composite materials, plants) should also be able to be measured in such a holder.
Required specification	- Hold multiple cells (and cell types) simultaneously (~50)

	- Hold/heat multiple different size of cells – wide/narrow rectangular, sandwich cells, holders for solid samples. - Temperature: -10-150 ± 0.1 °C - Controlled heating rate
Sharing possibilities	- Compatible with SKADI
Service requirements	- Water and/or glycol and/or oil bath for heating - Dry air for removing condensation (integrated include to the holder itself or as a separate device) - Heated/cooled through water bath, would like an internal thermometer and feedback-loop built-in.
Integration requirements	- x and y translation table. Should have fixed approximate coordinates for pos. 1. After fine alignment of pos. 1, input of these values should generate accurate values for all remaining positions. - Mounted on general sample table - Length in beam: <100 mm (longest snout)

NOTE: Recommend removing ambient sample holder included in earlier. Unless there is an advantage for more cells in the ambient cell holder or lighter/easier installation, then temperature stable holder should be used. Advantages: easier if users change their mind, never a bad thing to be able to specify the temperature.

ii. Sample changer with individual/isolated heating elements (priority = 2)

Scientific case	The ability to heat multiple samples to different temperatures simultaneously is ideal for samples that require long equilibration times (e.g. large samples) or slower heating rates (e.g. biomolecules), those that need to be heated over a wide range of temperatures (e.g. polymer gels, polymer nanocomposites). As well as for samples that can be destroyed/denatured at higher temperatures. For these samples it would be attractive to consecutively measure samples at different temperatures but not expose the entire sample set to all the temperature extremes. Specifically, this would be important for facilitating faster run times by avoiding time lost while the water bath/heating elements heats & cools.
Required specification	- Heat multiple cells simultaneously (>20) at different temperatures - Hold different cell types: wide/narrow cells, sandwich cells - Temperature: -10-150 ± 0.1 °C - Controlled heating rates
Sharing possibilities	- Compatible with SKADI
Service requirements	- Water and/or oil bath for cooling - Dry air for removing condensation

Integration requirements	- x and y translation table. Should have fixed approximate coordinates for pos. 1. After fine alignment of pos. 1, input of these values should generate accurate values for all remaining positions. - Mounted on general sample table - Length in beam: <100 mm (longest snout)

iii. Quartz cells of various dimensions (priority = 5)

Scientific case	Required for the large variety of soft matter samples to be measured on LoKI
Required specification	- Narrow rectangular cells (10 mm wide) with pathlengths of 1, 2 and 5 mm, with (~80%) and without stoppers (~20%) - Wide rectangular cells (20 mm wide) with thin glass walls (similar to narrow cells) and without feet to ensure proper thermal contact – may need to be custom made. - Care that the glass thickness and necks are standardised. (Large variation of neck sizes even within the same suppliers causes difficulties when loading/aligning samples)
Sharing possibilities	- LoKI should have its own set but should be compatible with SKADI
Service requirements	
Integration requirements	- All standard changers should hold the family of generic cells.

iv. Dismountable 'sandwich'-style cells (priority = 3)

Scientific case	Non-fluid samples, e.g. 'wet' gels, thin films, solid organic/biological samples, polymer melts, that can't be loaded into typical quartz cuvettes
Required specification	- 'Sandwich'-style dismountable brass cells, with round quartz windows held apart by rubber o-rings. - Work with sample apertures of up to 8 x 8 mm - Compatible with high temperatures (up to 350 °C)
Sharing possibilities	- LoKi and SKADI
Service requirements	
Integration requirements	- Should be able to fit into the thermostated cell holders.

v. Pumps (HPLC and syringe pumps) (priority = 3)

Scientific case	Large scale structures and macroscopic flow in realistic flow fields is a central research goal in complex fluids, including polymers, emulsions, surfactants, foams. Huge case to have a range of pumps available for stopped flow experiments, microfluidics, micro-rheology

	- A HPLC pump can maintain a constant flow of mobile phase through the system (or HPLC) regardless of back pressure. Ideal for flow cells. - Syringe pumps are a cheaper option for smaller microfluidic cell designs. Examples: Flow cell and entangled polymer melts: Science, 2003, 301, 1691
Required specification	- Heated sample wells and syringes – ideally their temperatures can be set independently of each other. - Ability to recover samples or collected in a waste container e.g.1: JASCO LC-4000 Series HPLC pumps, up to 700 Bar, flow rate of 5.0 mL/min, attachments available for solvent mixing. e.g.2: Braintree scientific BS-8000 syringe pumps for microfluidics that can be controlled through a Labview script. Accepts multiple syringe sizes
Sharing possibilities	- LoKi, SKADI, FREIA, ESTIA
Service requirements	- Water for cooling/heating - Compressed air
Integration requirements	- x & y translation for initial alignment and then fixed. - Integrated software or controllable through instrument software

vi. Stopped-flow cell with HPLC pump (priority = 3)

Scientific case	Stopped-flow method allows for rapid mixing within a millisecond and subsequent observation of the structural changes taking place. For SANS, typically scans are done in extremely short time scales and the measurement is repeated to improve statistics. The high flux on LoKI will either remove or reduce the number of repetitions required. Useful for monitoring self-assembled structures, 'biological' samples, nanoparticle growth, etc. Examples: Monitoring vesicle formation in situ: Colloid Polym. Sci., 2010, 288, 827
Required specification	- Heated sample wells and syringes – ideally their temperatures can be set independently of each other. - Heated sample position. - Variable SANS pathlength? - Offline alignment should be facilitated. - Initially samples recovered or collected in a waste container? - After washing through the cell, we need to ensure its clean – could use a similar mechanism to the biosaxs devices which use a small camera.
Sharing possibilities	- LoKi and SKADI

Service requirements	- Water in/out for cooling/heating - Sample recovery system or container for waste collection - Compressed air
Integration requirements	- x & y translation for initial alignment and then fixed. Course offline alignment ideally and then wheeled in/lifted into the sample position. - Software integrated into NICOS - Mounted on general sample table - Length in beam (before detector tank): <200 mm (longest snout)

vii. Goniometer (priority = 3)

Scientific case	A goniometer for grazing-incidence SANS to study structures that exist both in the plane of the film and normal to the substrate, e.g. for polymer thin films, multilamellar lipid bilayers, colloidal crystals. The device would also be useful for mounting and aligning flow experiments.
Required specification	- Slit set needs to be carefully considered. - Huber stack at SANS2D (ISIS-TUI Berlin collaboration). Translation in the x and y directions, 2 circle segment and a circle goniometer can be used together. For GiSANS – JJ X-ray neutron slights can be mounted before the Huber stack to allow the beam size to be varied. - Mounting need to be set such that positioning relative to beam centre and centre of rotation are highly reproducible and easy to align. - Ideally it will be possible to isolate the goniometer within a chamber to control the atmosphere e.g. gas, humidity, temperature. Discuss radius of goniometer, cabling and motors.
Sharing possibilities	- Potentially between LoKi, SKADI, FREIA, ESTIA. However others are likely to have gonimeters permanently installed.
Service requirements	- If the stage could be loaded into some kind of atmospheric chamber, air, pressure, gases, temperatures could be varied.
Integration requirements	- Reproducible positioning crucial due to fiddly requirements with alignment. - Two (small) beamstops for the direct and reflected beam. - Mounted on general sample table. - Length in beam (before detector tank): <200 mm (longest snout)

General case for flow-SANS and rheo-SANS

As stated in the outline, LoKI is ideally suited to studying dynamic systems, which change their structure in solution over short periods of time. Although these changes can be induced by a range of internal and external influences, after temperature, the second most popular type of "dynamic" experiment is likely to involve flow or rheology. Such studies will take full advantage of the high flux (small sample apertures) and large simultaneous q-range at LoKI, therefore are considered crucial for facilitating early and general science. General topics measured using these techniques include: hydrogels, polymer/nanoclay systems, polymer melts and blends, emulsions, membrane phases, wormlike micelles, soft colloids e.g. block copolymer micelles, biological samples.

viii. Rheometer (priority = 4)

Scientific case	SANS of samples under stress in the 1,3- and 2,3-planes, radial and tangential, respectively. Examples: Hydrogels for tissue analogues: Macromol. Biosci. 2018. 18, 1800018 Heat responsive gels: karen edler, SAXS, J. Colloid Interface Sci. Surfactants: Takeda, Langmuir, 2011, 27, 1731
Required specification	- Sample aperture slits mounted to the front of the rheometer like NIST(?). Entry and exit markers for alignment - Temperature: -10-200 ± 0.1 °C - Shear rates: 0.001 – 1500 s^{-1} - Need to consider titanium versus quartz cups and a couple of different pathlengths
Sharing possibilities	- LoKi and SKADI
Service requirements	- Compressed air, access to liquid nitrogen cylinder, electronics, external connection to laptop outside of the sample area
Integration requirements	- Translation in y, then fixed. Translation in x during measurement. - Time-stamping and integration of rheometer software - Mounted on its own trolley or general sample table. - Length in beam (before detector tank): <200 mm (medium snout)

ix. Dielectric Rheometry* (priority = 2)

Scientific case	SANS of samples under stress in the 1,3- and 2,3-planes (radial and tangential), combined with simultaneous measurement of impedance, rheology and SANS particularly charged colloidal dispersions, proteins, ionic surfactants, nanocomposites. Examples: Worm-like micelles: Riley, Soft Matter, 2018, 14, 5344
Required specification	- Modified forced-convection oven. Titanium cup and bob for neutron transmission and serve as the two electrodes for AC dielectric spectroscopy. Induction, capacitance and resistance (LCR) meter for performing spectroscopy. - Sample aperture slits mounted to the front of the rheometer **Adaption of standard rheometer should be possible.*

Sharing possibilities	- LoKi and SKADI
Service requirements	- Compressed air, access to liquid nitrogen cylinder
Integration requirements	- Time-stamping and integration of rheometer and LCR meter software. - Mounted on general sample table. - Length in beam (before detector tank): <250 mm (medium snout)

x. Magnetic Rheometry* (priority = 1)

Scientific case	SANS of magneto-rheological fluids under stress in the 1,3- and 2,3-planes (radial and tangential).
Required specification	- Applied fields up to 1 T, sample temperatures: 10-170 °C. - Sample aperture slits mounted to the front of the rheometer - TA have the MR set-up available as an accessary. Not sure if it is suitable for SANS **Adaption of standard rheometer should be possible*
Sharing possibilities	- LoKi and SKADI
Service requirements	- Compressed air, access to liquid nitrogen cylinder
Integration requirements	- Time-stamping and integration of rheometer software. - Mounted on general sample table. - Length in beam (before detector tank): <250 mm (medium snout)

xi. 1,2-plane shear cell (priority = 2)

Scientific case	Microstructures of solutions that exhibit shear banding, a phenomenon that can only be investigated by the resolving the structure along the 1,2-plane (velocity gradient direction). These experiments yield the degree of structural anisotropy and direction of the anisotropy. Such systems include worm-like micelles that have significant impact in industrial formulations. Examples: WLM micelles & rheo SANS: Soft Matter, 2009, 5, 3858.
Required specification	- Such a cell may be need to be custom built. Nice example at NIST [J. Vis. Exp., 2014, 84, e51068]. Anton Paar are also working on one.
Sharing possibilities	- LoKI and SKADI
Service requirements	- Compressed air, access to liquid nitrogen cylinder
Integration requirements	- Slits? Need the ability to scan to be able to spatially resolved measurements along the velocity gradient directions. - Time-stamping and integration of rheometer software.

	- Mounted on general sample table. - Length in beam (before detector tank): <250 mm (medium snout)

xii. Couette Shear Cell (rotating outer cylinder) (priority = 2)

Scientific case	Samples requiring much higher sheer rates e.g. polymer-clay hydrogels,
Required specification	- Temperature: 10-100 °C - Variable shear rates, e.g. 0.001 – 1500 s^{-1} - Quartz inner and outer cylinders. - Rotation speeds: 1-3000 rpm; Speed rates: 5-15000 s^{-1} - Device is already available at NIST and RAL (with limited oscillary shear)
Sharing possibilities	- LoKI and SKADI
Service requirements	- Compressed air
Integration requirements	- Steady shear measurement should be directly controllable through the instrument software - Mounted on general sample table. - Length in beam (before detector tank): <200 mm (medium snout)

xiii. Rotating/tumbler cell holders (priority = 5)

Scientific case	Rotating cells are extremely useful for resuspending sedimenting particles. Any experiments with large particles, such as colloidal suspensions and for crystalline and powdered samples. Slowly rotating samples continuously provides more uniform conditions than periodic shaking or inversion.
Required specification	- Slowly tumble/rotate samples so that there is no net velocity. - Temperature: 10-100 °C - Independent tumbling speeds (is this necessary?) - Require a minimum of 2 or 3 cells for commissioning Nice example: Olsson et al, Meas. Sci. Technol., 2013, 24, 105901
Sharing possibilities	- LoKI and SKADI
Service requirements	- Power supply for motor and heating element, air cooling
Integration requirements	- x and y translation table. Should have fixed approximate coordinates for pos. 1. After fine alignment of pos. 1, input of these values should generate accurate values for all remaining positions. - Mounted on general sample table - Length in beam: <100 mm (long snout)

xiv. 2.2 or 3 Tesla magnet (priority = 3)

Scientific case	The high flux at LoKI and short run times could be particularly beneficial for properly measuring 'training effects' and scanning hysteresis loops, with the ability to go through more cycles at a constant temperature. Samples include magnetic nanoparticles, ferrofluids (magnetite nanoparticles), etc.
Required specification	- Magnetism: 0-3 Tesla - Sample changer rack that 'slides' the samples through the magnet centre (or a robot) - Ability to scan accurately through the range of magnetic fields. - Bio-applications, e.g. magnetic nps for drug delivery may want accurate temperatures up to and including 37 °C. - Water-cooled or RT to 150 °C holders - Sufficiently large pole gap e.g. 100 mm will be required for some users, however this leads to a compromise with uniformity of fields - Maximum possible scattering angle from the sample (min. 40° in at least some directions)
Sharing possibilities	- *ESS pool of SEE*
Service requirements	- Requires long semi-rigid flex-lines coming out of the head connected to a compressor. - Gas handling system - Dewar - ISIS 7.5 T cryomagnet and frame assembly like SANS2D suggested - Example: Goudsmit electromagnet requires 48-60 V d.c. at 435-650 A and demineralised cooling water supply at 22-25 l/min at 5 bar.
Integration requirements	- Expensive and expect it to be rarely used on LoKI, therefore it is critical that this can be shared between LoKI and SKADI. - Care to be taken for magnetic joints/connections in the stacks - Length in beam (before window to detector): <350 mm (medium snout) - Top access to the sample area

NB: I don't think this will be highly required for LoKI – magnetic experiments are not typically high throughput and don't benefit as much from a large simultaneous q-range – but should be available but would probably be better served on SKADI.

xv. 1 Tesla electromagnet with high frequency (priority = 1)

Scientific case	Stroboscopic measurements – modulating fields. The ability to ramp on/ramp off could be useful for ferromagnets, however these go through cycles slowly (hours at the fastest).

Required specification	- Sample changer rack that 'slides' the samples through the magnet centre. - Sufficient pole gap e.g. 100 mm
Sharing possibilities	- LoKI, SKADI, FREIA, ESTIA
Service requirements	- Ability to cycle on and off magnetic fields at high frequencies - Requires long semi-rigid flex-lines coming out of the head connected to a compressor. - Gas handling system - Dewar - ISIS 7.5 T cryomagnet and frame assembly like SANS2D suggested
Integration requirements	- Care to be taken for magnetic joints/connections in the stacks - Length in beam: <350 mm (medium snout)

xvi. Cryomagnet (priority = 2)

Scientific case	Occasional experiments may require the cryomagnet (a part of ESS pool of SEE), although not part of the LoKI science case and would be *rarely used*. 17T : Protein crystal growth, diamagnetism, self-assembled structures and liquids crystals, flux lattices (falling into soft matter) 11 T : as above but more flexible scattering geometries 7 T : as above, presumably smaller, easier set-up and sufficient for the general user case of LoKi
Required specification	- Sample changer rack that 'slides' the samples through the magnet centre (or robot) - Up to 17 T - Temperatures down to a couple of Kelvin.
Sharing possibilities	- *ESS pool of SEE*
Service requirements	- Requires long semi-rigid flexlines coming out of the head connected to a compressor. - Gas handling system - Access to liquid nitrogen dewar - Cryostat and frame assembly like SANS2D - CCR compressor
Integration requirements	- Critical that this can be shared between LoKI and SKADI. - Care to be taken for magnetic joints/connections in the stacks - Entire structure should be wheeled/ or craned in from the ground level up. Chicane required to feed in supplies.

	- Cave design will try to incorporate a Sample Environment Labyrinth if possible - Length in beam: <500 mm (short snout) RARELY USED.

xvii. Humidity cell / chamber (priority = 2/3 depending on first science)

Scientific case	There are multiple examples that experiments which will require controlled humidity, e.g. fuel cell membranes (proton exchange membranes), lipid bilayers, filter membranes, semi-crystalline polymers.
Sharing possibilities	- LoKI, SKADI, might be compatible for FREIA, ESTIA?
Required specification	- Humidities: 3- 95% (±1%) as a minimum initial requirement. - Temperatures: 10–100 °C. Feedback loop between RH and temperature desirable. - Transparent windows (e.g. quartz) - Speed of RH control and tuneability - FYI: Hygrostatic solutions range from 2-98.5% and 5-80 °C. - Multiple samples positions would be desirable Nice example at NIST: Jackson, Rev. Sci. Instrum., 2013, 84, 075114
Service requirements	- Humidity pumps to 'flush' through the vapour pressure generating a flow of humid air past the sample. Ideally, we would also have an isolated chamber for isolated humidities. - Gas inlets and power supply.
Integration requirements	- Length in beam (before detector tank): <200 mm (shortest snout) - Mounted on general x/y translation sample table.

xviii. High pressure cell (priority = 2)

Scientific case	High pressure SANS measurements would include studying the phase behaviour of proteins, biomolecules, surfactants, polymer super-critical fluids, super critical CO_2-water microemulsions
Required specification	- Max pressure: up to 5 kbar (example at ILL) - Temperature: -10-200 °C - Water channels for cooling - For liquid and solid samples - Perform fast pressure jumps - Liquid samples up to 500 MPa [Rev. Sci. Instrum 2007, 78, 125101]
Sharing possibilities	- LoKI, SKADI, might be compatible for FREIA, ESTIA?
Service requirements	- Cooling water

	- Compressed air
Integration requirements	- Mounted on general x/y translation table - Length in beam: <250 mm (medium snout)

xix. Cryostat (priority =2)

Scientific case	Occasional experiments may require the cryostat (a part of ESS pool of SEE), although might be rarely used on LoKI
Required specification	Generally, allowing temperatures down to 1 or 2 K with electromagnetic attachments Multiple different options at other facilities: - 3He insert (Tmin = 270 mK) - ILL orange cryostat (Tmin = 1.5 K) - Cryo free dilution refrigerator - Displex CCR (Tmin = 4K) Likely to be decided from what other instruments require.
Sharing possibilities	- *ESS pool of SEE* (but needs thin windows for SANS)
Service requirements	- Gas handling system - Liquid nitrogen dewar - Cryostat and frame assembly like SANS2D - CCR compressor
Integration requirements	- Wheeled or craned in. - Length in beam: <500 mm (short snout)

xx. Furnace (priority = 2)

Scientific case	Some systems will require much higher temperatures than are possible with the standard thermostated holders, e.g. up to 1000 °C.
Required specification	- Maximum temp: 1000 ± 0.1°C - Positions for 10-20 solid samples with independent temperature control - Controlled heating rates up to 100°C per minute - Vacuum - Heated windows to prevent condensation - ILL style furnaces?
Sharing possibilities	- *ESS pool of SEE* (but needs thin windows for SANS)
Service requirements	- Vacuum pump - Cooling water

	- Inert gases
Integration requirements	- Mounted on general sample table - Length in beam: <200 mm (medium snout)

xxi. Linkam Temperature Stage (priority = 2)

Scientific case	Rapid heating and cooling with accurate control for polymers, metals, ceramics, biological materials, polymer films for photovoltaics
Required specification	- Temperature: -200 to 600 °C < 0.1 °C - Max heating rate increase 150 °C/min - Min heating rate increase 100 °C/min
Sharing possibilities	- LoKI only
Service requirements	- Liquid nitrogen &/or for cooling - Compressed air
Integration requirements	- Mounted on general sample table - Length in beam: <100 mm (long snout)

xxii. Ultrasound transducers (priority = 2 - but I think it could be cool initial science).

Scientific case	Anything that undergoes cavitation under sonification. Such ultrasonic devices are common tools in laboratory and industrial settings to produce cavitation events for cleanings, emulsification, cell lysis, food science
Required specification	Two nice examples at NIST: 1. Low and high intensity ultrasound at mixed frequencies. Fixed and varying the frequency, up to 3 MHz. [Soft Matter, 2018, 14, 5283] 2. Smaller sample cell which fits inside standard sample cell environments allowing for variation of temp, humidity and magnetic fields. Option to vary sample thickness. Dimensions: 25 x 25 x 30 mm^3. [Rev. Sci. Instrum., 2018, 89, 015111.] *REQUIRES DEVELOPMENT WORK*
Sharing possibilities	- LoKI only
Service requirements	
Integration requirements	- Length in beam (before detector tank): <100 mm (longest snout) - Mounted on general x/y translation table - Potentially designed to fit in generic thermostated cell holders. - Isolation table?

xxiii. Support for *in operando* battery and fuel cell measurements (priority = 2)

Scientific case	In operando battery and fuel cells experiments are popular but generally require a lot of ancillary equipment which should be supported.
Sharing possibilities	- *ESS pool of SEE*
Required specification	- Cells will be user supplied
Service requirements	- Potentiostat for multiple cell types
Integration requirements	- Would benefit from a round sample aperture. The battery cells typically have small windows which are always circular, therefore suffer from a loss of available flux with square apertures. - Length in beam: <100 mm (longest snout) - Mounted on general x/y translation table

xxiv. Stress/stretching rig for soft matter

Scientific case	Investigation of deformed gels, tensile deformation of proton exchange membranes under immersed and thermal conditions.
Required specification	- Thermostated reservoir so the sample can be suspended in the required solvent. - Nice example: Tensile stress of fuel cell membrane, Rev. Sci. Instrum., 2013, 84, 105115
Service requirements	- Mineralised water - Condensed air
Integration requirements	- Mounted on general x/y translation table - Length in beam: <200 mm (medium snout)

xxv. Inline spectroscopy (priority = 3)

Scientific case	The observation of chemical processes directly with SANS measurements, has become increasingly desirable as we aim for a deeper understanding of any underlying processes and interactions which might affect the nanostructure formed. These studies are particularly crucial for dynamic systems, to ensure sample stability, purity, chemical conditions, and where it is not possible to perform further measurements or characterisation on intermediate states ex situ. e.g. for biomacromolecules, surfactants, polymers
Required specification	An ideal device would include a variety of characterisation devices: e.g. Raman, UV/Vis absorption, fluorescence and FTIR spectroscopies, conductive, tubidity and pH measurements which all already exist independently at SAXS beamlines and some SANS beamline. Jackson, Rennie et al. have work underway on a fluorimeter, densiometer, UV/Vis spectrometer combined with a stop-flow cell.

	ILL example: Sci. Rep., 2018, 8, 7299
Service requirements	
Integration requirements	- Length in beam: <100 mm (long snout)

xxvi. Sample changer robot (priority = 3, although how it may be integrated into the sample area is a high priority, e.g. chicane hatch to post samples or cartridges)

Scientific case	As the power at ESS increases, and the measurement times decrease, there will be an increasing demand/necessity for high throughput SANS experiments. However, although automated set-ups already exist at X-ray beamlines, there are a few extra considerations that need to be accounted for here, e.g. larger sample volumes, deuterated solvents should ideally be kept in sealed containers, high neutron flux could lead to "hot" sample holders/cells
Required specification	Two options that could be considered: 1. Current BioSAXS automatic sample changer robots which can transfer up to 200 μL which might be feasible for us? Controlled sample temperature for exposure and storage compartment. Ability to perform in situ mixing – could it be set up to mix 100% D_2O and 100% H_2O solution in the required ratios for contrast matching experiments? e.g. Arinax bioSAXS 2. Remote handling of stoppered sample cells. A new cartridge of cells would be loaded externally, placed in the sample area and then each cell is loaded by a robot into the sample position. *REQUIRES DEVELOPMENT WORK*
Service requirements	-
Integration requirements	- Additional sample area available for sample changer robot (~1 m^2) - Device could become very hot after a run. May need remote handling to change then sample cartridges. At high flux will the sample cartridges may need to be replaced remotely. i.e. without opening up the full sample area. - Appropriate masking/shielding needs to be checked, can't simply use the current x-ray models. - Chicane hatch through wall to post samples or cartridges

xxvii. Dynamic light scattering (priority = 2)

Scientific case	*In situ* monitoring of samples which are prone to aggregating over time, e.g. biomolecules. Static light scattering could also be of interest.
Required specification	DLS set-ups are already available at ISIS, ILL, and JCNS.

Sharing possibilities	- LoKI only
Service requirements	- External laptop for software
Integration requirements	- Laser: will need its own PSS/integration with the interlock systems - Length in beam: <200 mm (medium snout)

xxviii. Size-exclusion chromatography (priority = 1)

Scientific case	Allow SANS to be measured from freshly purified sample material. Ideal for the study of unstable biological molecules (e.g. proteins), where aggregation or denaturation is a major problem. This is now a standard set-up on bioSAXS instrumentation. This would be low priority for LoKI if there is going to be a dedicated bioSANS beamline.
Required specification	Size-exclusion chromatography system to separate particles by size. Uv-vis absorption spectrometer to confirm purity SEC-SANS on D22: J. Appl. Cryst., 2016, 49, 2015
Sharing possibilities	- LoKI only
Service requirements	
Integration requirements	- Length in beam: <150 mm (long snout)

Other ancillary measurements (priority = 1):
- Differential scanning calorimetry
- Isothermal scanning calorimetry

5. Sample Area

5.1 Requirements

- A rigid (semi-permanent?) sample table with x and y translations for the smaller sample environments, which can be locked into place when needed using the custom designed mounting system. This mounting system should also lock into place the larger sample environments (e.g. magnets, cyrostats).
- Cabinet for deactivating samples and sample holders
- Julabos
- Safety: PSS system, oxygen monitors, no gap left behind by sliding door, air conditioning, sprinklers, web cams
- Room for laptop inside the sample area.
- Cave design should try to incorporate a sample environment labyrinth
- Collimation snout:
    - Snout lengths need to be able to support the range of sample environment sizes with 100 mm flexibility provided by the extendable snout section.

    - Crashing and motion control protection.
    - Narrow snouts to fit 'into' complex sample environments.

5.2 **Future considerations**

- Vibration stages
- Room for robotic handling of stoppered cells
- Robotic preparation of solutions
- Gap through sample wall to exchange samples without opening the cave.

5.3 **Sample area supplies**

- containment exhaust
- access/feedthrough for liquid nitrogen
- demineralised water
- dry compressed air
- Gases: argon, helium, nitrogen
- Ethernet
- waste collection

Also need cable labyrinth for external electronics and user provided equipment, e.g. connection to external laptops/potentiostats, control units