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LoKI - A Broad Band High Flux SANS Instrument for the ESS

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Abstract. The European Spallation Source (ESS) will be a long pulse 5MW spallation neutron source built in Lund, Sweden. It is expected that 7 out of a final suite of 22 instruments will enter commissioning in 2019/2020, with the remainder coming online by 2025. LoKI is a SANS beamline designed primarily with the needs of the soft matter, bio-science and materials science communities in mind. The trend in all of these fields is towards complexity and heterogeneity. These factors are manifested both spatially and temporally and so high flux, small beam sizes and a wide simultaneous Q range are required. We are thus constructing a 10 m + 10 m SANS instrument with the sample position 22.5 m from the source. Using the full ESS pulse length of 2.86 ms and two pairs of choppers, this provides a wavelength band of 7 Å at 14 Hz or 17.5 Å at 7 Hz whilst maintaining reasonable resolution. The resolution can be enhanced by generating four shorter sub-frames with an optional series of additional choppers. Combining this configuration with variable beam collimation and multiple banks of detectors covering a large solid angle, maximal use is made of the flux available from the ESS source and measurements with over 3 orders of magnitude in simultaneous Q range are possible.

1. Introduction

The European Spallation Source (ESS), currently under construction in Lund, Sweden, aspires to be the world's leading facility for research using neutrons, with unprecedented source brightness and intensity [1]. The ESS will be a long pulse spallation neutron source with a pulse length of 2.86 ms and a repetition rate of 14 Hz [1]. A total of 22 instruments or beamlines will be operational or in commissioning by the end of 2025 with 7 entering commissioning in 2019/2020. Since 2011, the ESS has been managing the development of instrument concepts by university groups and research institutions across Europe, and by in-house scientists based in Lund. The choice of instruments is through an ongoing process of annual proposal calls and review by expert panels. The proposal for LoKI [2] was submitted in October 2012 and approved for construction in October 2013. Here we outline the conceptual design of the instrument with some reference to possible technical solutions.

2. Scientific Goals

Small angle neutron scattering is a technique that is applied across a spectrum of scientific disciplines, with users from chemistry, physics, biology, materials science, engineering and geoscience. LoKI is designed primarily with the needs of the soft matter, biophysics and materials science communities in mind and the trend in all of these fields is towards complexity and heterogeneity.

Complexity manifests itself in the study of multi-component systems studied as a function of multiple environmental conditions (e.g. pressure, temperature, shear, magnetic field) simultaneously. In order to be able to examine the possible parameter space, a combination of faster measurements, measurements on smaller sample volumes, and measurements with a good signal-to-noise ratio is required.

Heterogeneity is seen both spatially and temporally. Spatial heterogeneity is manifested as different structure at different length scales, from the nanometre scale to the millimetre scale. This can be driven by applied stimuli such as shear and flow [3], electrical or magnetic fields, or by intrinsic structural features of the material. Examples of the former are shear banding in surfactant systems [4] and the flow re-orientation of polymers. Examples of the latter are nano-composite materials, multi-component gels [5, 6, 7], and porosity in rocks [8, 9, 10, 11]. To address this spatial heterogeneity requires a wide Q range to examine the sub-micrometre length scales and small beams to examine the heterogeneity on the millimetre scale. Furthermore, since these heterogeneities are often driven by non-equilibrium conditions, the accessible Q range must be measured simultaneously.

Temporal heterogeneity is seen in the form of stimulus-response experiments (e.g. shear relaxation), in the kinetics of formation of materials when the components of the material are mixed (e.g. mixed micelle formation)[12, 13] and in the growth of biomolecule aggregates such as fibrils. In order to examine these systems with sufficient time resolution a high neutron flux is required and a wide simultaneous Q range is needed.

Not only are the systems of interest becoming more complex and heterogeneous, but they are also becoming smaller in volume. Examples of this are the small amounts of protein complexes that can be purified and deuterated, thin film systems such as organic photovoltaics, and bio-mimetic or polymer membranes. In these cases it is vital that the instrumental background be as low as possible in order to discern the small scattering signal obtained.

The ability to reach Q values above the typical 0.8 to 1.0 Å^{-1} opens up significant areas of new science when combined with wide-angle scattering studies and the rapidly advancing fields of materials simulation. The study of, for example, ionic liquids and their ordering in the presence of solutes calls for the combination of SANS, wide-angle scattering and atomistic or coarse-grained molecular dynamics simulations. The analysis techniques used in biological solution scattering, such as ab-initio shape reconstruction, require data out to high Q as do studies of nano-composite materials where the size of the particles or domains may be only a few nanometres.

Non-equilibrium studies often use complex sample environments and require strong integration of the sample environment with the neutron measurement in order to tie sample conditions tightly to the measured scattering. Space is also required for the use of in-situ complementary measurement techniques, for example light or x-ray scattering, or UV spectroscopy simultaneously with the neutron scattering measurement. LoKI has a flexible sample area that can be easily re-tooled for different experiments through the use of interchangeable sample environment platforms.

Consultation with the user community and advice from expert panels lead to the development of top level requirements that encapsulate the scientific needs discussed above:

- The instrument shall allow data to be collected to a Qmin of < 0.001 Å^{-1}.
- The instrument shall allow data to be collected to a Qmax of > 2 Å^{-1}.

- The instrument shall allow data to be collected simultaneously over a continuous Q range with Qmax/Qmin > 1000.
- The instrument shall match the size of the neutron beam to the size of the sample.
- The instrument should allow the Q resolution (dQ/Q) to be optimised for the experiment.
- The instrument should be capable of providing a Q resolution < 10% dQ/Q over the whole Q range.
- The instrument should allow data collection from samples < 8 mm^3 volume
- The instrument should maximise the signal-to-background (S/B) ratio of the small angle scattering.

3. Instrument Overview

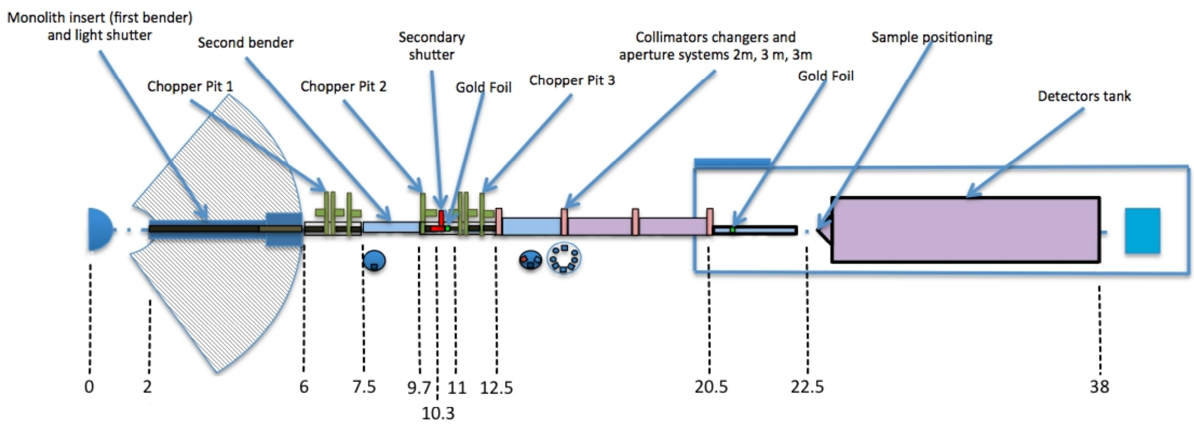


Figure 1. Layout of the LoKI instrument.

The instrument begins at 2 m from the source with a 4 m long bender to close line-of-sight by the 6 m position. The first chopper pit houses the bandwidth selection chopper pair at 6.5 m and the first resolution enhancement chopper at 7 m. A second 2.1 m long bender closes line-of-sight a second time between the first and second chopper pits. The second chopper pit houses the second resolution enhancement chopper at 10 m from the source. There is then a straight guide to the third chopper pit which houses the frame-overlap chopper pair at 11.5 m and the final resolution enhancement chopper at 12 m. The variable collimation begins at 12.5 m with the first aperture wheel, followed by: a 2 m long guide changer drum; the second aperture wheel at 14.5 m; a 3 m long guide changer drum; the third aperture wheel at 17.5 m; a 3 m long guide changer drum; and the final aperture wheel at 20.5 m. There is then a variable length evacuated flight tube between the final aperture wheel and the sample aperture, with the sample position at 22.5 m from the source. The detector system, for which there are two options, is then mounted following the sample. The two options for detector geometry are (Figure 5): (1) a "window frame" arrangement of three detector banks; and (2) a "barrel" arrangement where the detector vessel is lined with detector banks running parallel to the beam axis and a high-resolution rear detector is placed perpendicular to the beam axis for the lowest angles. In both cases the rear detector is moveable along the beam axis. The sample position and detector system are housed in the instrument cave which is constructed of steel "cans" filled with borated wax.

The instrument design has initially been optimised to make use of the recently conceived "pancake" moderator that the ESS is planning to use [14, 15]. This moderator produces a cold spectrum and has a viewable face of 3 cm high × 12 cm wide.

4. Optics

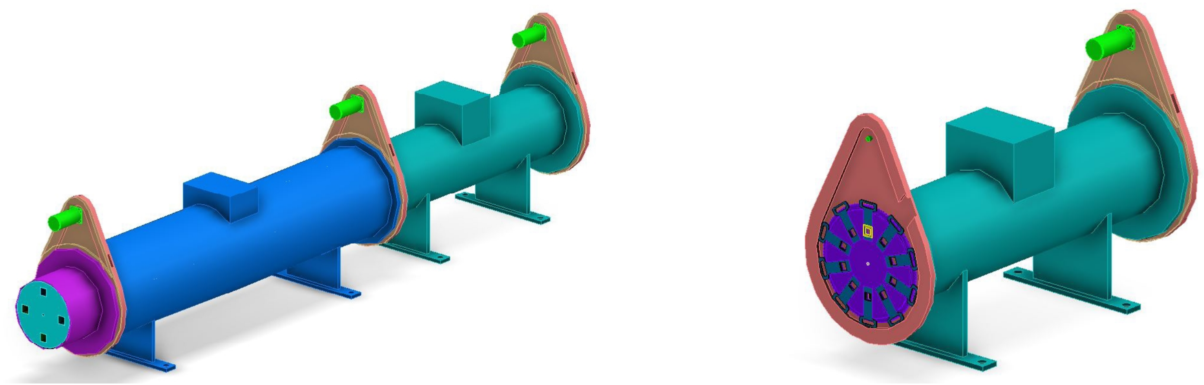
4.1. Line-of-sight

In order to minimise background and avoid the prompt spike of high energy neutrons produced when the proton beam hits the target, the instrument is designed to have the start of the collimation two times out of line-of-sight of the source. One times line-of-sight closure is achieved when no point at the exit of a section of the instrument has a direct line-of-sight to the start of that section. The first line-of-sight closure is designed as being at the outer wall of the target monolith, at 6 m from the source. The second line-of-sight closure takes this point as its start and is closed at the second chopper pit.

Several guide geometry options have been considered in developing the concept for the neutron optics. Monte Carlo simulations using Vitess [16] were used to assess the relative performance of the different options. Horizontal and vertical bends, both s-bends and continuous curves, were considered and the guide dimension in the direction of the bend was allowed to vary to minimise the curvature and potentially increase the transmission whilst maintaining line-of-sight closure. An additional requirement was that the guide be straight within the chopper pits and thus the lengths of the two benders were fixed at 4 m and 2.1 m respectively.

The result was that a horizontal s-bend was the most favourable, having a first bender, 4 m in length, 2.5 cm wide × 3 cm high with a radius of 66.0 m and a second bender, 2.1 m in length, 2.5 cm wide × 3 cm high with a radius of 36.8 m. Thus the guide is asymmetric in shape from the start of the optics at 2 m until the end of the second chopper pit. The guide then expands from 2.5 cm × 3 cm to 3 cm × 3 cm between the second chopper pit and the start of the collimation. All of the guides in the collimation section are 3 cm × 3 cm.

4.2. Collimation



(a) (b)

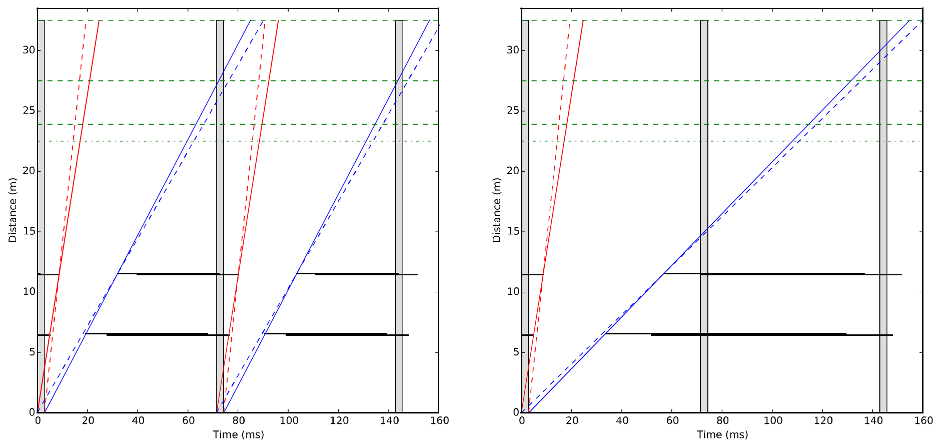
Figure 2. The variable collimation system consisting of Collimation Drums (Figure 2a (section shown)) and Aperture Wheels (Figure 2b (shown connected to collimation drum)).

The variable collimation section provides for source-to-sample distances of 2 m, 5 m, 8 m and 10 m. The three longest distances can be matched with a corresponding sample-to-detector distance through moving the rear detector. The collimation system consists of three drums (Figure 2a) that allow for switching between guide and an empty tube lined with neutron absorbing material. A spare empty tube is provided for future upgrades and a blocked position is provided as a means of blocking the neutron beam if the secondary shutter is inoperable. At the ends of each collimation section are aperture wheels (Figure 2b) that provide 10 possible aperture choices to allow the collimation to be tuned to the sample size and resolution required by the experiment.

5. Chopper System

5.1. Bandwidth Selection

Wavelength selection and frame overlap prevention is performed using two double-disc choppers. The first chopper, located at 6.5 m from the source, has two co-rotating discs, each with a 120° opening. This provides for an adjustable chopper aperture through variation of the phasing between the two discs. The second chopper, located at 11.5 m from the source, is identical to the first and provides the frame overlap suppression.



(a) (b)

Figure 3. Time-distance diagrams for Mode 1 (14Hz) (Figure 3a) and Mode 2 (7 Hz) (Figure 3b). Detector positions for a window-frame type layout are indicated with long dashes. Short dashes show the sample position.

LoKI provides two modes of operation offering different wavelength bands and hence different Q ranges. Mode 1 has the choppers running at 14 Hz. To access the wavelength band from 3 Å to 10 Å (2.0 Å to 11.0 Å with penumbra), an open time of 14.5 ms is required as seen in Figure 3a. The timing of the chopper with respect to the source can be adjusted such that a different range of wavelength is selected, for instance moving the whole band to longer wavelength. This allows the scientist to select for lower Q values whilst still using every pulse from the source. Such operation will also improve the wavelength resolution, as longer wavelengths will be used.

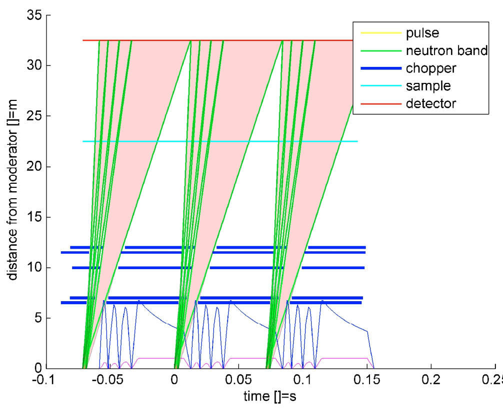
Mode 2 has the choppers running at 7 Hz. This allows access to the wavelength band from 3 Å to 18.5 Å (2.0 Å to 19.5 Å with penumbra), using every other source pulse as shown in Figure 3b. In order to achieve this range whilst still completely filling the frame the open time of the choppers must be adjusted, by changing the phasing of the discs, to be longer than twice that of 14 Hz operation.

5.2. Resolution Enhancement

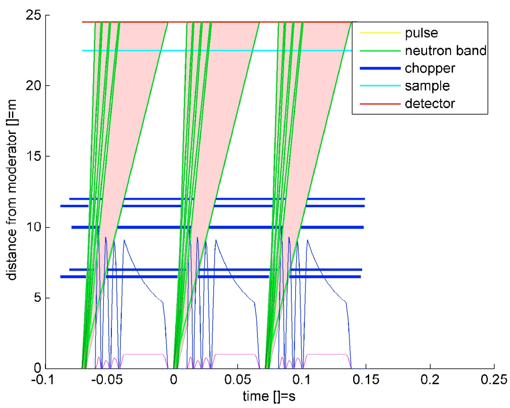
The instrumental resolution dQ/Q is limited by the time-of-flight resolution of the shortest wavelengths that contribute to a given Q bin. In the default operation mode, dT is fixed at the pulse length of 2.86 ms. At the shortest detector distance, using 2 Å neutrons, this gives a dT/T of 27%. This value adds in quadrature with the other components of the resolution [17], but will dominate the resolution at high Q. LoKI will enable two approaches to enhancement of Q resolution.

The first of these is through the use of neutron event recording, which identifies the time of arrival of each neutron at the detector. LoKI, along with all ESS instruments, will allow the scientist to determine the data binning scheme post experiment and it will be possible to exclude short wavelength neutrons from the data reduction and do so selectively as a function of Q. This is valuable for materials such as block-copolymer blends where there are strong peaks in the data that require high resolution but the inter-peak scattering is of lower intensity and so requires more neutron counts but can make use of lower resolution. In particular there is a need to have good Q resolution at high Q, for example in studies of fibres, liquid crystals or multi-lamellar systems such as lipid or surfactant vesicles. The ability to make use of longer wavelength, higher time resolution, neutrons at high angles will be key to being able to make use of post-measurement resolution tuning. This also demands a large solid angle of detectors and detectors at high angles.

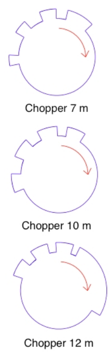
The second approach is to employ a system of choppers to reduce the virtual length of the source pulse for the case of shorter wavelength neutrons [18]. This allows for approximately a threefold improvement in the resolution of the short wavelength frames. Whilst the integrated flux on sample is reduced using this method compared to using the full pulse at all wavelengths, it is equivalent to a flux increase at a given resolution obtained by rejecting short wavelengths in the data reduction using the method above. This frame multiplication method is therefore of most use when resolution enhancement over the whole Q range is required, rather than selective enhancement, for example in the case of solving the structures of biological macromolecules in solution.



(a)



(b)



(c)

Figure 4. Time-distance diagrams with resolution enhancement choppers in place. Figure 4a shows the effect of the choppers with 10 m collimation. Figure 4b shows their effect with 2 m collimation. Figure 4c shows the chopper disc arrangement that produces the frame multiplication.

6. Detectors

The traditional approach of using ^{3}He detectors is no longer a viable option for ESS instruments, owing to the limited availability of ^{3}He, its high cost [19, 20, 21] and that some detector requirements cannot be fulfilled using this technology [22]. Thus an alternative neutron technology solution based on ^{10}B is introduced for this application. Boron carbide ($^{10}B_4C$)

thin-film detectors are currently being developed by several groups worldwide and are proven to be a reliable and promising replacement for ^{3}He detectors ([23, 24, 25, 26, 27, 28]).

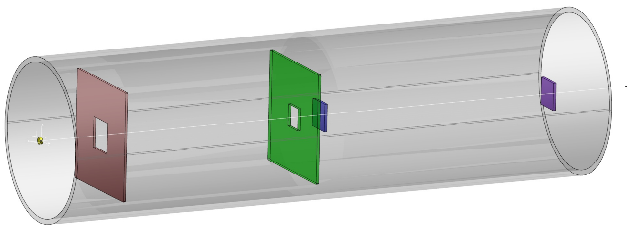
6.1. Window Frame

The window frame detector geometry option consists of a series of three detector panels with holes in centre of the first two. In this way a large solid angle can be covered simultaneously. These detector banks are placed within a large vacuum vessel, and the sizes of the panels are designed to minimise the size of that vessel whilst still meeting the requirements for scattering angle coverage. Thus, the front and middle panel are 2.0 m $\times$ 2.0 m and the rear detector is 0.5 m x 0.5 m. Square holes are left in the centre of the front and middle panels to allow full illumination of the detectors behind. The front, middle and rear detectors have resolutions of 15 mm, 8 mm and 3 mm respectively.

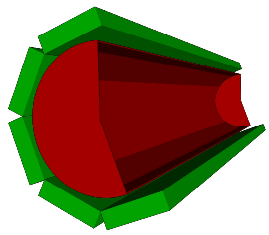
The panels will utilise ^{10}B coated detection planes placed at an inclined angle in either a BAND (Boron Array Neutron Detector) or Multi-Blade [29] arrangement. The preferred BAND design makes use of boron coated alumina lamellae, a GEM system for signal multiplication and a padded anode for event location.

6.2. Barrel

The barrel detector geometry option has been described elsewhere [30, 31] and consists of ^{10}B coated panels lying parallel to the beam direction around the outside of an evacuated or gas filled tube. This geometry maximises the path length of neutrons through the boron conversion layer, whilst keeping it thin enough to allow escape of the conversion products. The inclined geometry allows the wire pitch to be 10 mm along the whole length of the tube whilst maintaining adequate angular resolution.



(a)



(b)

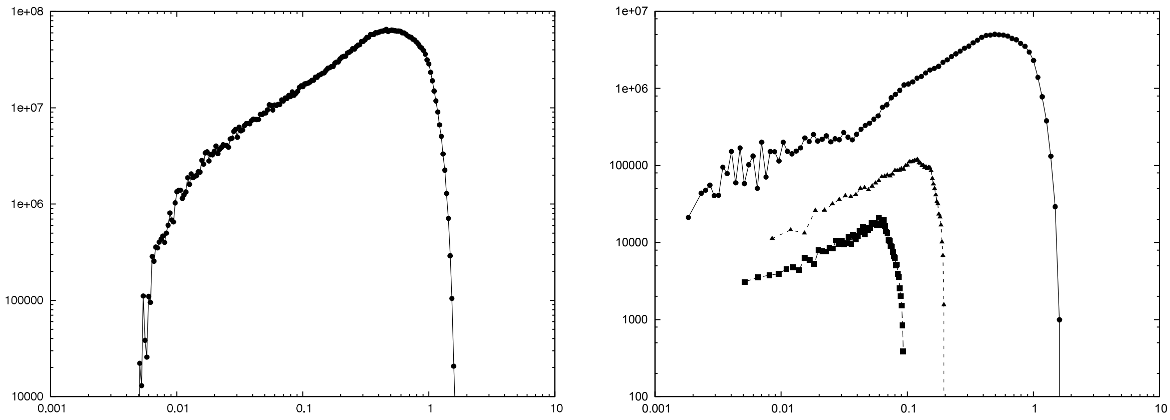
Figure 5. Possible detector geometry configurations for LoKI, as they appear in the instrument proposal. Figure 5a shows the “window-frame” geometry inside a vacuum tank, while Figure 5b depicts the “barrel” geometry.

7. Performance

Monte Carlo simulations using McStas [32, 33] have been performed with the window-frame detector geometry. Using circular apertures and setting the source aperture to be twice the diameter of the sample aperture the flux at sample can be obtained and some values are shown in Table 1. In terms of flux on sample, LoKI will provide more than an order of magnitude increase over existing instruments and deliver a wide simultaneous Q range as shown in Figure 6.

8. Conclusion

Our initial work indicates that a world-leading SANS instrument can be built at the ESS making maximum use of the new moderator geometry. The instrument design will be completed in 2015/2016 and the instrument will enter hot commissioning with neutrons in 2019/2020.



(a) (b)

Figure 6. Simulated elastic scattering from water at 2 m (Figure 6a) and 10 m (Figure 6b) collimation lengths with 20 mm diameter source and 10 mm diameter sample apertures (●) compared with simulation of 10 m (■) and 5 m (▲) collimation settings on D22.

Table 1. Flux at sample from Monte Carlo simulations as a function of collimation.

L1 (m)	A_1 diam (mm)	A_2 diam (mm)	Flux ($n/s/cm^2$)
2	20	10	1.4×10^9
5	20	10	2.5×10^8
10	20	10	1.1×10^8
2	10	5	1.1×10^8
5	10	5	3.0×10^7
10	10	5	6.4×10^6

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