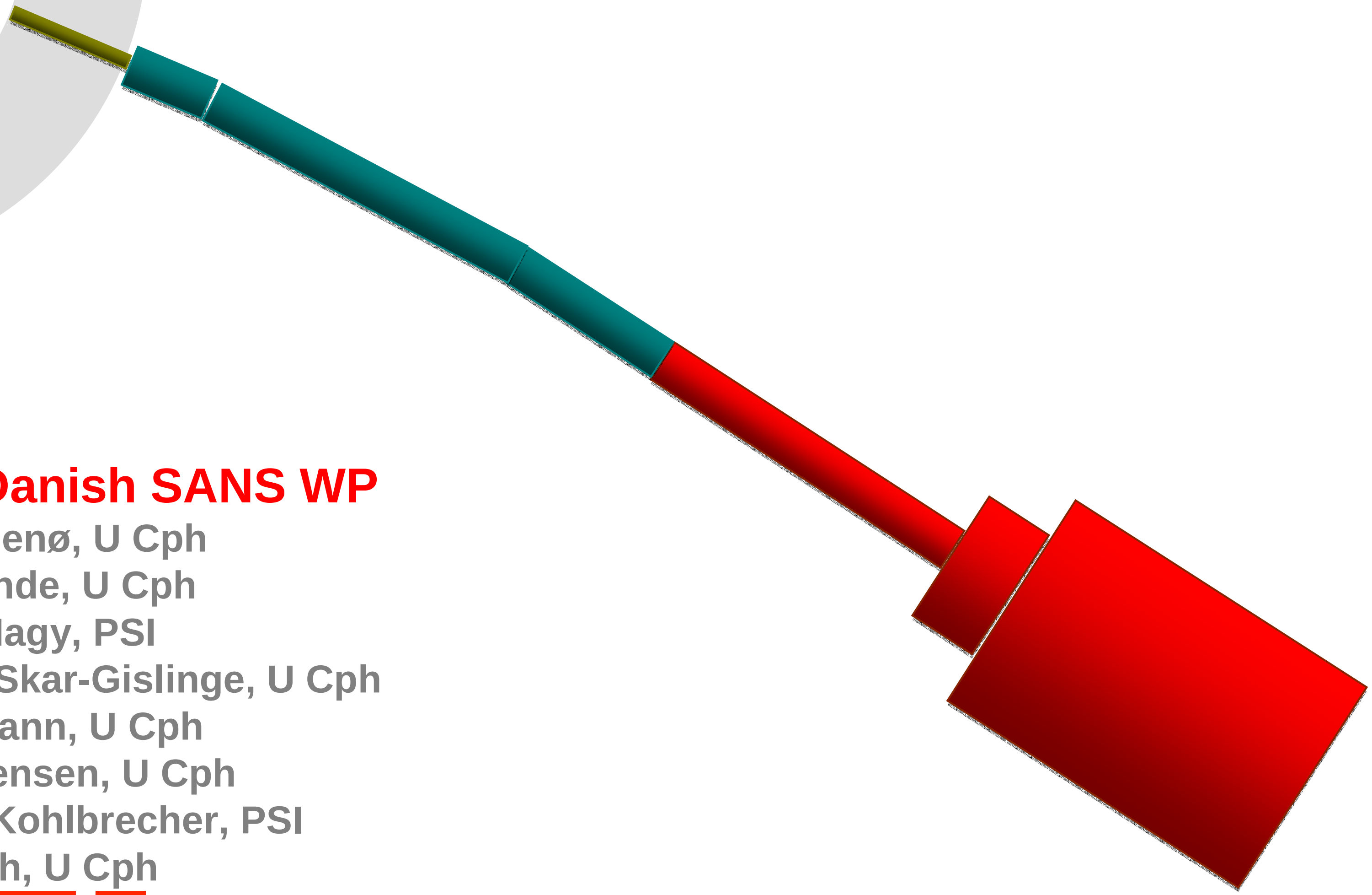
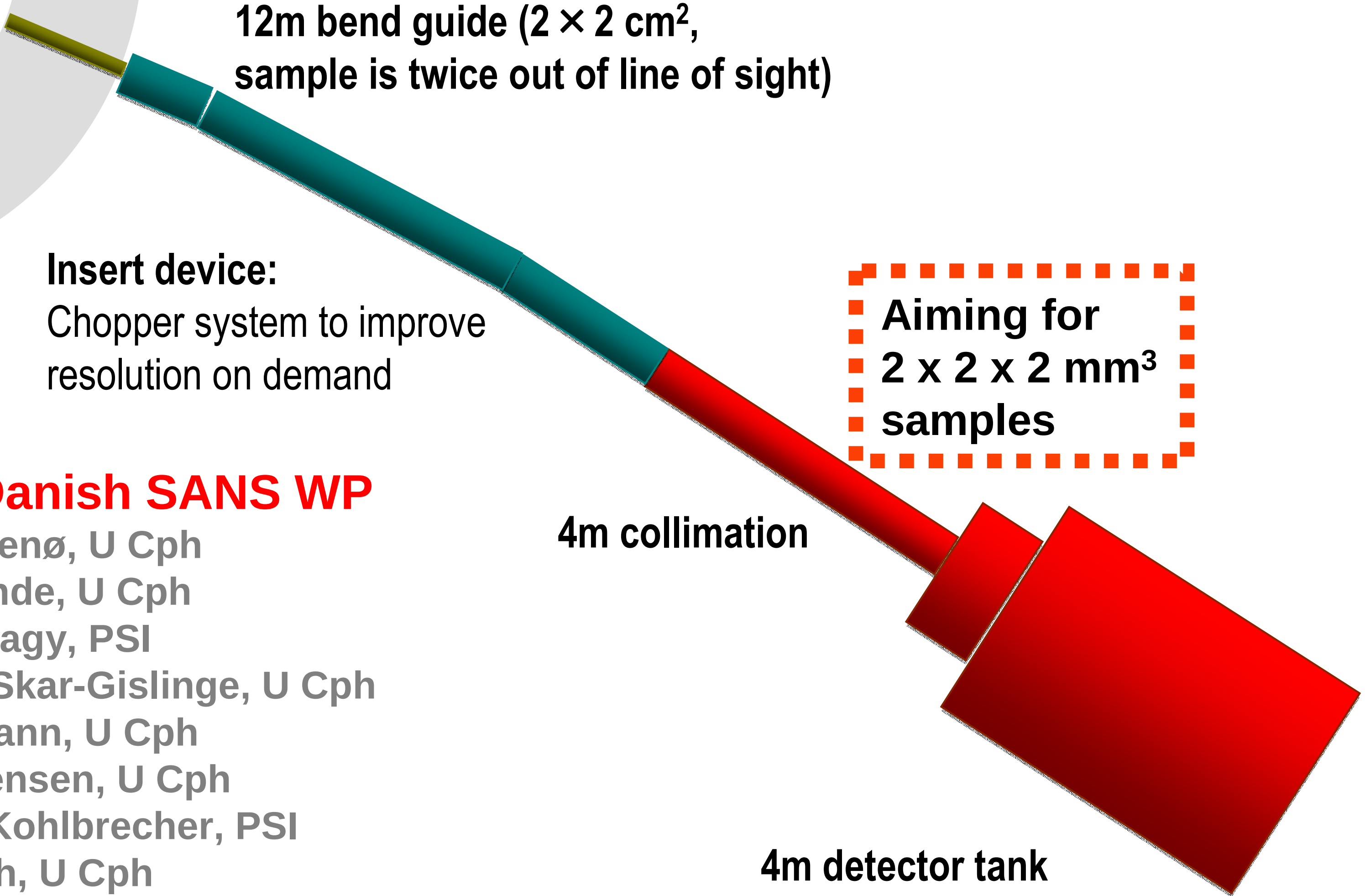
Compact SANS optimized for high flux and small sample volumes



Swiss-Danish SANS WP
Kaspar Klenø, U Cph
Søren Kynde, U Cph
Gergely Nagy, PSI
Nicholas Skar-Gislinge, U Cph
Kim Lefmann, U Cph
Kell Mortensen, U Cph
Joachim Kohlbrecher, PSI
Lise Arleth, U Cph

ESS

Compact SANS optimized for high flux and small sample volumes

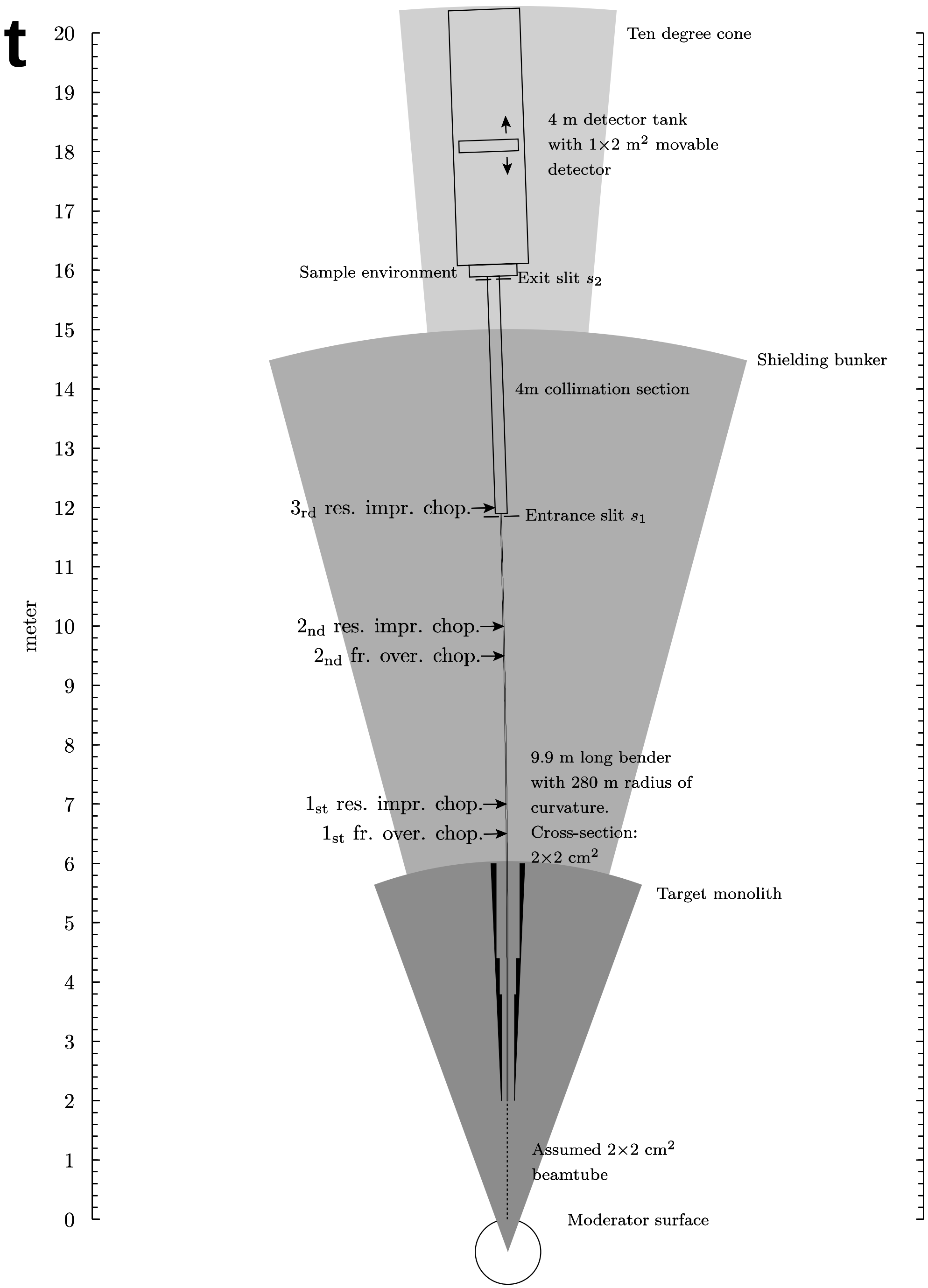


Swiss-Danish SANS WP
Kaspar Klenø, U Cph
Søren Kynde, U Cph
Gergely Nagy, PSI
Nicholas Skar-Gislinge, U Cph
Kim Lefmann, U Cph
Kell Mortensen, U Cph
Joachim Kohlbrecher, PSI
Lise Arleth, U Cph

ESS

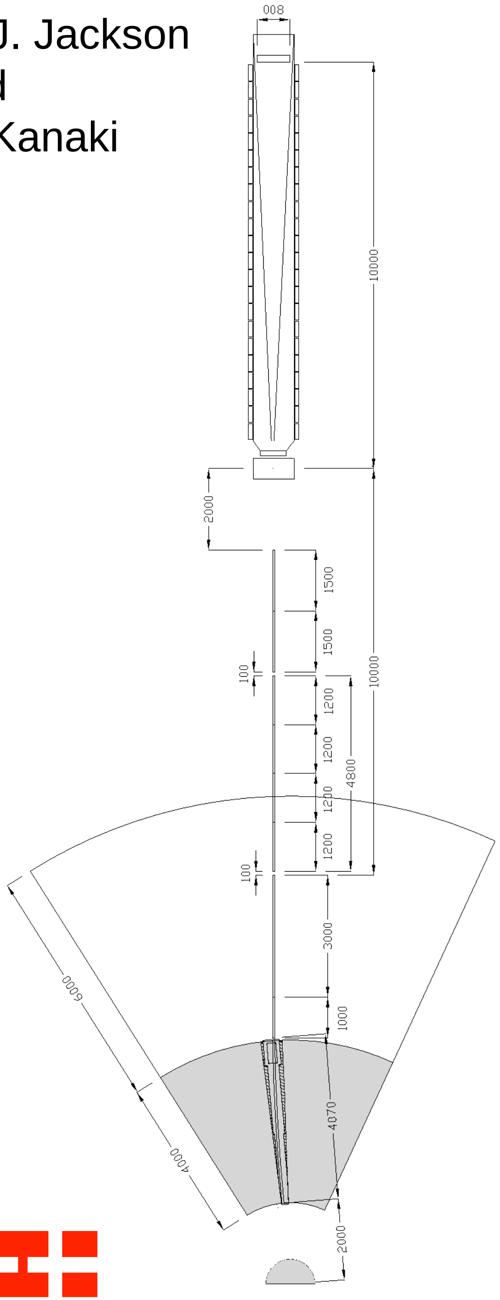
The proposed instrument

- 12 m curved guide to block line of sight twice
  ~95% of the neutron flux is transferred through the guide
- Up to 4 m Collimation
- Up to 4 m Sample-detector distance
- Frame overlap choppers and resolution improving choppers placed inside the shielding bunker.
- Sample environment placed right outside the shielding bunker at 16 m from the source.
- Detector is a 1×2 m² detector. (5mm pixels. Preferably 2 mm pixels near center)
- Resolution improving choppers allow for trading flux for wavelength resolution on demand

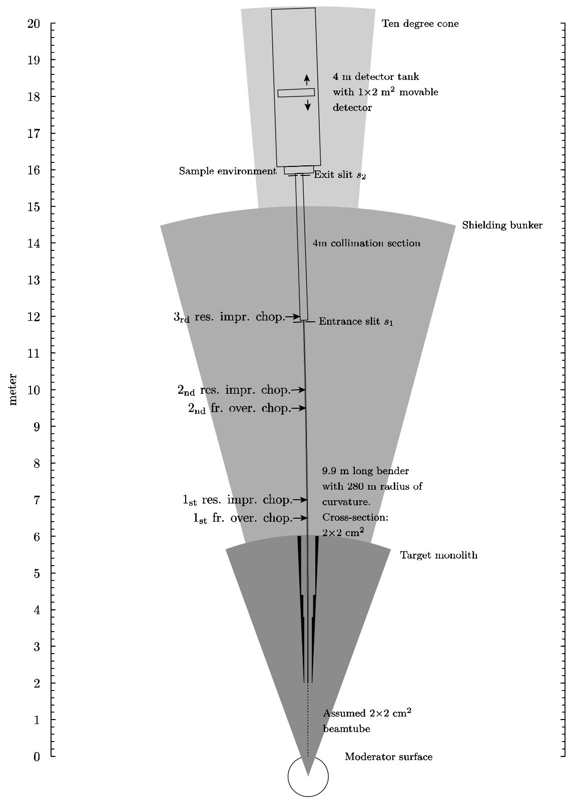


LoKI

A. J. Jackson
and
K. Kanaki

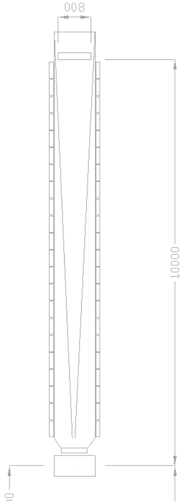


Compact SANS

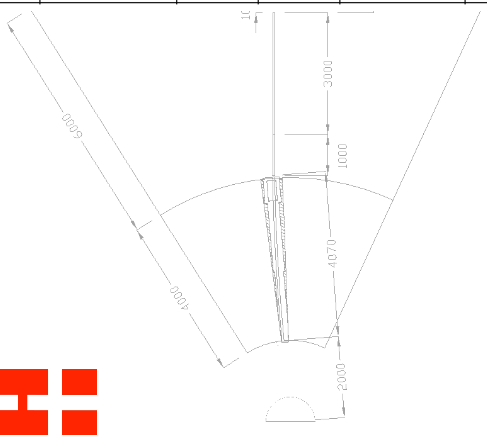


LoKI

A. J. Jackson
and
K. Kanaki



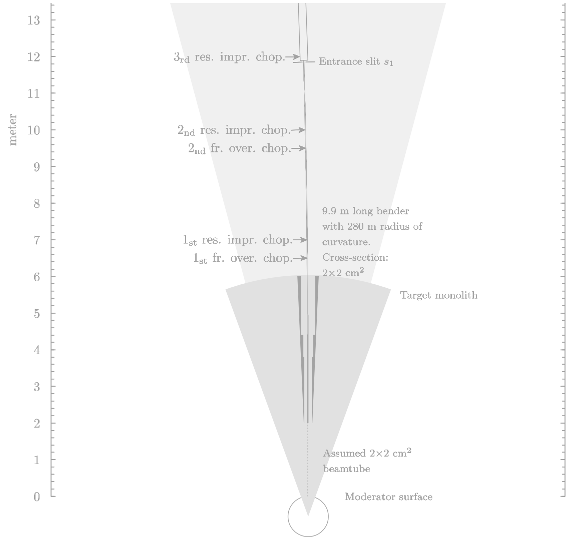
Ap1 Diam (mm)	Ap2 Diam (mm)	L1 (m)	L2 (m)	Beam Size (mm)	Min Q (Å⁻¹)	Flux (n/cm2/s)
20	10	2	5	85	7.28E-03	3.87E+08
10	5	2	5	43	3.64E-03	9.67E+07
4	2	2	5	17	1.45E-03	1.55E+07
20	10	5	5	40	3.43E-03	6.19E+07
10	5	5	5	20	1.71E-03	1.55E+07
4	2	5	5	8	6.85E-04	2.48E+06
20	10	10	10	40	2.09E-03	1.55E+07
10	5	10	10	20	1.05E-03	3.87E+06
4	2	10	10	8	4.19E-04	6.19E+05



Compact SANS

Instrument length: $L = A + L_1 + L_2$	q_{min} ($Å^{-1}$)	q_{max} ($Å^{-1}$)	Flux on sample (n/s/cm^2)	Neutrons on 50.3 mm^2 sample (n/s)
17=15+1+1	0.0080	1.27 (2.02)	12×10^8	5.9×10^8
18=14+2+2	0.0042	0.71 (1.38)	3.3×10^8	1.7×10^8
20=12+4+4	0.0023	0.37 (0.78)	0.88×10^8	0.44×10^8
ILL D22 A+2+2	0.0168	0.47	0.28×10^8	0.11×10^8

Table 2: *Instrument performance with the Large Sample configuration: $s_1=8$ mm, $s_2=4$ mm and 1×1 m^2 detector. Numbers in parenthesis correspond to the 2×1 m^2 detector*



LoKI

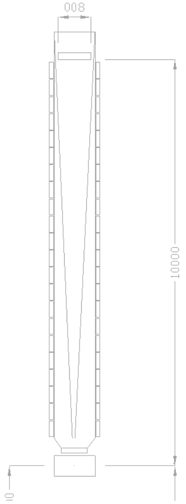
A. J. Jackson
and
K. Kanaki

Compact SANS

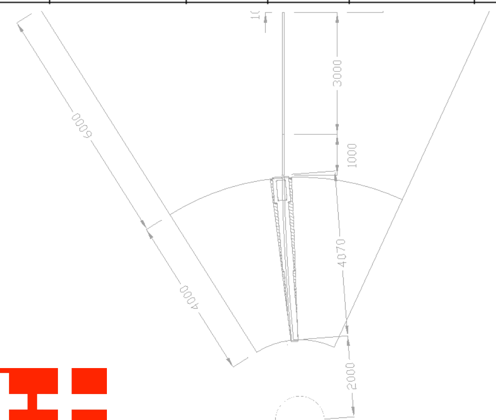
Flux

$1.55\text{x}10^7 \longleftrightarrow 3.3\text{x}10^8\ /4$

$1 \longleftrightarrow 5.3$

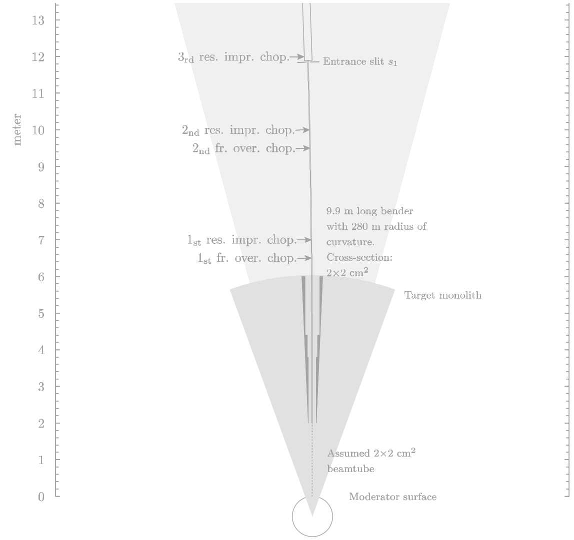


Ap1 Diam (mm)	Ap2 Diam (mm)	L1 (m)	L2 (m)	Beam Size (mm)	Min Q (Å^{-1})	Flux (n/cm2/s)
20	10	2	5	85	7.28E-03	3.87E+08
10	5	2	5	43	3.64E-03	9.67E+07
4	2	2	5	17	1.45E-03	1.55E+07
20	10	5	5	40	3.43E-03	6.19E+07
10	5	5	5	20	1.71E-03	1.55E+07
4	2	5	5	8	6.85E-04	2.48E+06
20	10	10	10	40	2.09E-03	1.55E+07
10	5	10	10	20	1.05E-03	3.87E+06
4	2	10	10	8	4.19E-04	6.19E+05



Instrument length: $L = A + L_1 + L_2$	q_{min} (Å^{-1})	q_{max} (Å^{-1})	Flux on sample (n/s/cm^2)	Neutrons on 50.3 mm^2 sample (n/s)
17=15+1+1	0.0080	1.27 (2.02)	12×10^8	5.9×10^8
18=14+2+2	0.0042	0.71 (1.38)	3.3×10^8	1.7×10^8
20=12+4+4	0.0023	0.37 (0.78)	0.88×10^8	0.44×10^8
ILL D22 A+2+2	0.0168	0.47	0.28×10^8	0.11×10^8

Table 2: *Instrument performance with the Large Sample configuration: $s_1=8$ mm, $s_2=4$ mm and 1×1 m^2 detector. Numbers in parenthesis correspond to the 2×1 m^2 detector*



LoKI

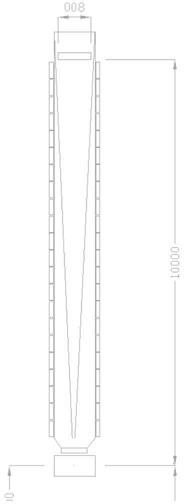
A. J. Jackson
and
K. Kanaki

Compact SANS

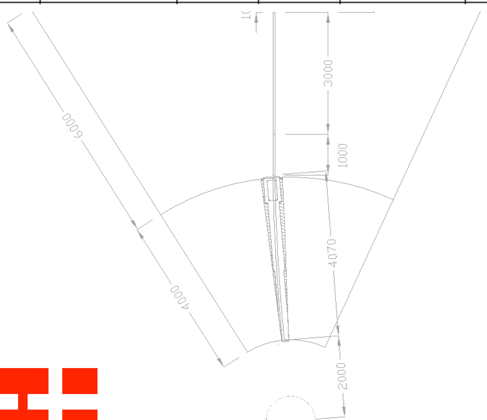
Flux

$1.55\text{x}10^7 \longleftrightarrow 3.3\text{x}10^8$ /4

$1 \longleftrightarrow 5.3$

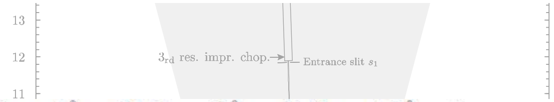


Ap1 Diam (mm)	Ap2 Diam (mm)	L1 (m)	L2 (m)	Beam Size (mm)	Min Q (Å^{-1})	Flux (n/cm2/s)
20	10	2	5	85	7.28E-03	3.87E+08
10	5	2	5	43	3.64E-03	9.67E+07
4	2	2	5	17	1.45E-03	1.55E+07
20	10	5	5	40	3.43E-03	6.19E+07
10	5	5	5	20	1.71E-03	1.55E+07
4	2	5	5	8	6.85E-04	2.48E+06
20	10	10	10	40	2.09E-03	1.55E+07
10	5	10	10	20	1.05E-03	3.87E+06
4	2	10	10	8	4.19E-04	6.19E+05

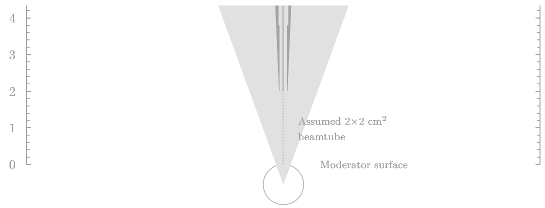


Instrument length: $L = A + L_1 + L_2$	$q_{\min}$ (Å^{-1})	$q_{\max}$ (Å^{-1})	Flux on sample (n/s/cm^2)	Neutrons on 50.3 mm^2 sample (n/s)
17=15+1+1	0.0080	1.27 (2.02)	12×10^8	5.9×10^8
18=14+2+2	0.0042	0.71 (1.38)	3.3×10^8	1.7×10^8
20=12+4+4	0.0023	0.37 (0.78)	0.88×10^8	0.44×10^8
ILL D22 A+2+2	0.0168	0.47	0.28×10^8	0.11×10^8

Table 2: *Instrument performance with the Large Sample configuration: $s_1=8$ mm, $s_2=4$ mm and 1×1 m^2 detector. Numbers in parenthesis correspond to the 2×1 m^2 detector*



L_1 (m)	$d\lambda/\lambda$ at 4Å	$d\lambda/\lambda$ at 8Å	$d\lambda/\lambda$ at 12Å	flux on sample (n/s/cm^2)
1	17%	8%	6%	12×10^8
2	16%	8%	5%	3.3×10^8
4	14%	7%	5%	0.88×10^8

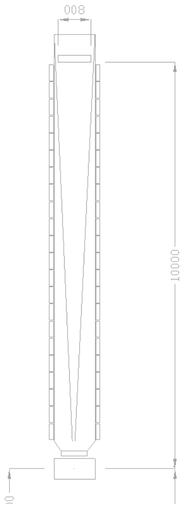


ESS

LoKI

A. J. Jackson
and
K. Kanaki

Compact SANS

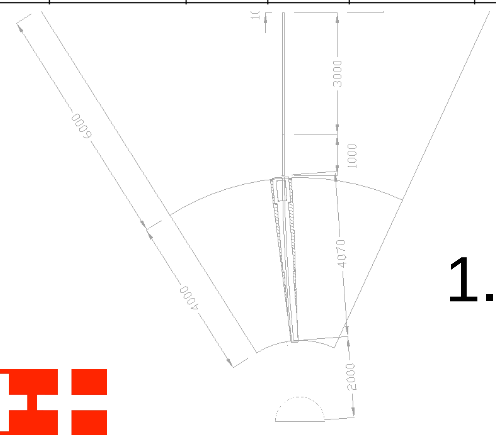


Flux

$1.55\times10^{7} \longleftrightarrow 3.3\times10^{8}$ /4

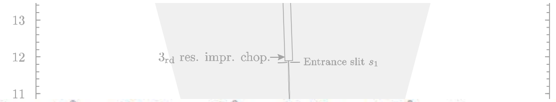
$1 \longleftrightarrow 5.3$

Ap1 Diam (mm)	Ap2 Diam (mm)	L1 (m)	L2 (m)	Beam Size (mm)	Min Q ($Å^{-1}$)	Flux (n/cm2/s)
20	10	2	5	85	7.28E-03	3.87E+08
10	5	2	5	43	3.64E-03	9.67E+07
4	2	2	5	17	1.45E-03	1.55E+07
20	10	5	5	40	3.43E-03	6.19E+07
10	5	5	5	20	1.71E-03	1.55E+07
4	2	5	5	8	6.85E-04	2.48E+06
20	10	10	10	40	2.09E-03	1.55E+07
10	5	10	10	20	1.05E-03	3.87E+06
4	2	10	10	8	4.19E-04	6.19E+05

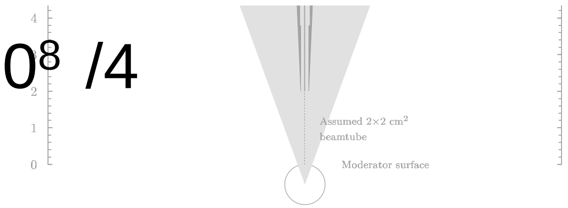


Instrument length: $L = A + L_1 + L_2$	$q_{\min}$ ($Å^{-1}$)	$q_{\max}$ ($Å^{-1}$)	Flux on sample (n/s/cm^2)	Neutrons on 50.3 mm^2 sample (n/s)
17=15+1+1	0.0080	1.27 (2.02)	12×10^8	5.9×10^8
18=14+2+2	0.0042	0.71 (1.38)	3.3×10^8	1.7×10^8
20=12+4+4	0.0023	0.37 (0.78)	0.88×10^8	0.44×10^8
ILL D22 A+2+2	0.0168	0.47	0.28×10^8	0.11×10^8

Table 2: *Instrument performance with the Large Sample configuration: $s_1=8$ mm, $s_2=4$ mm and 1×1 m^2 detector. Numbers in parenthesis correspond to the 2×1 m^2 detector*



L_1 (m)	$d\lambda/\lambda$ at 4Å	$d\lambda/\lambda$ at 8Å	$d\lambda/\lambda$ at 12Å	flux on sample (n/s/cm^2)
1	17%	8%	6%	12×10^8
2	16%	8%	5%	3.3×10^8
4	14%	7%	5%	0.88×10^8
1	9%	8%	6%	4.7×10^8
2	8%	8%	5%	1.3×10^8
4	7%	7%	5%	0.34×10^8



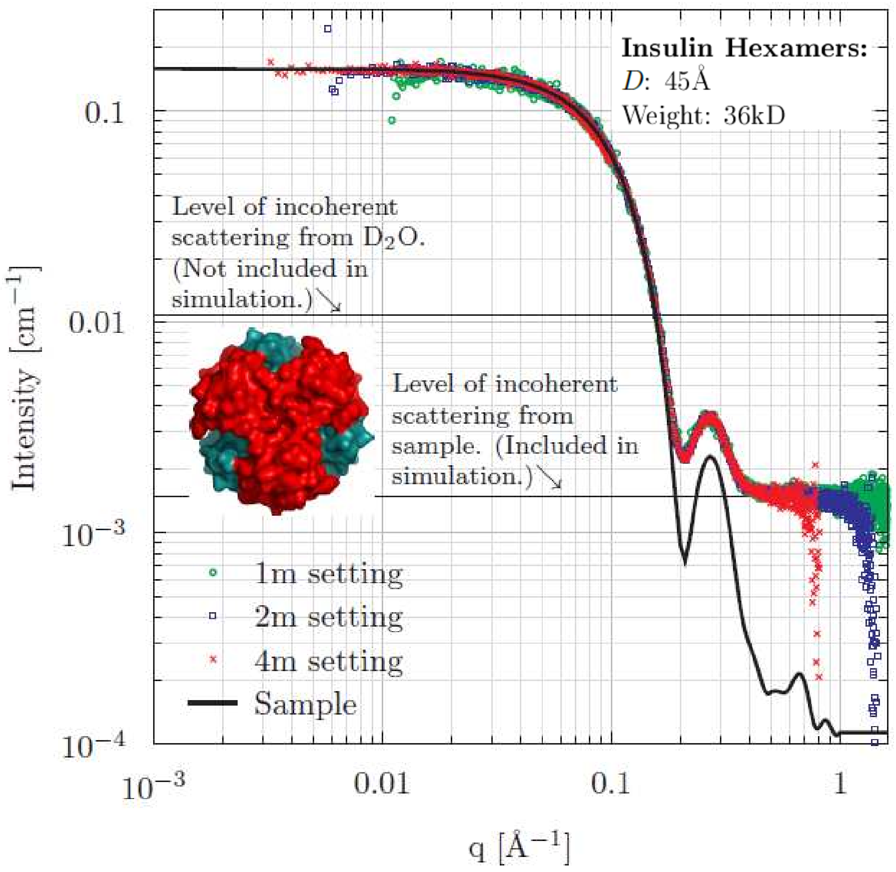
$1.55\times10^{7} \longleftrightarrow 1.3\times10^{8}$ /4

$1 \longleftrightarrow 2.1$

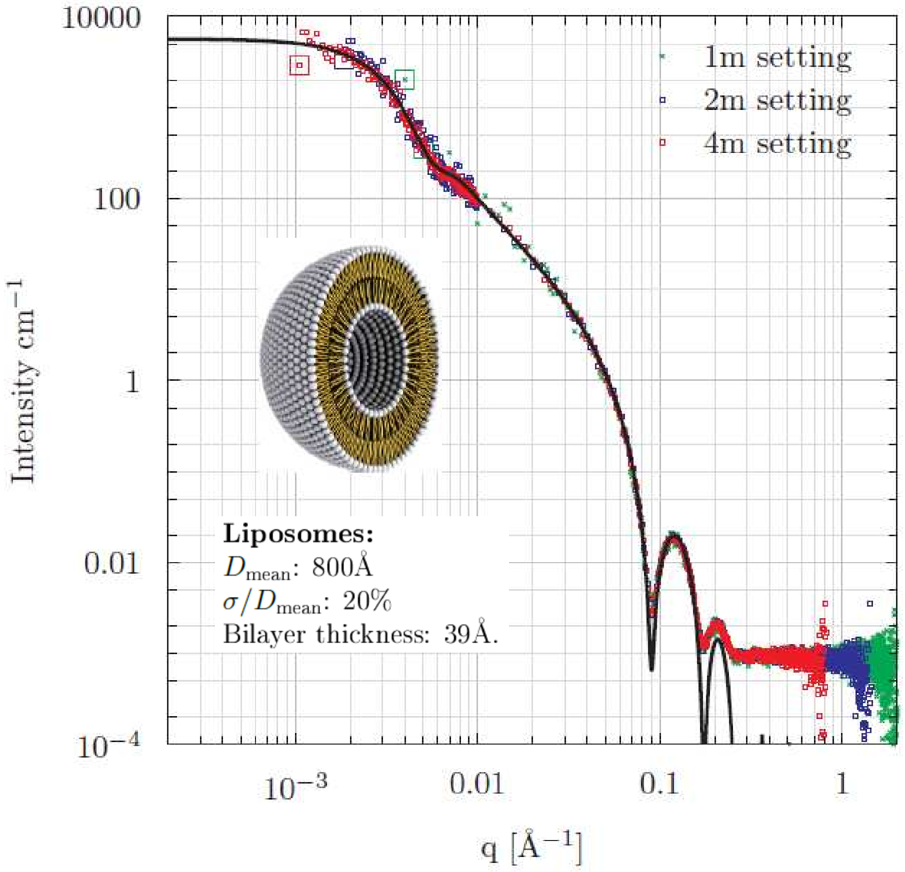
ESS

Example for the type of samples the instrument is optimised for.

s_1=8mm, s_2=4mm



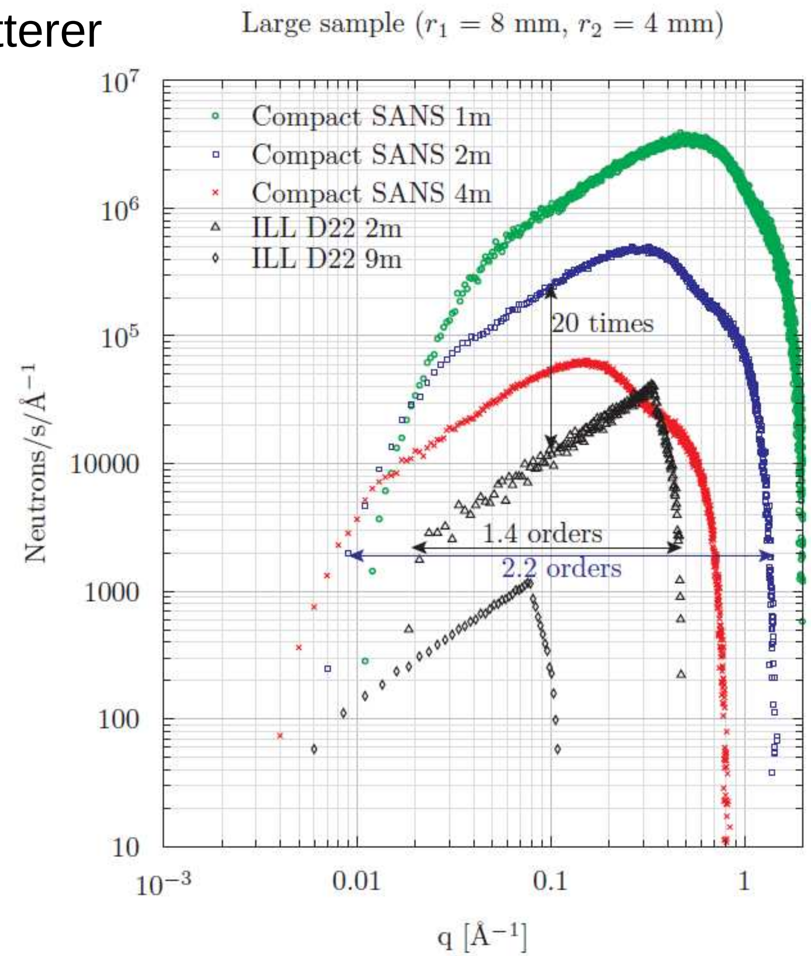
s_1=2mm, s_2=1mm

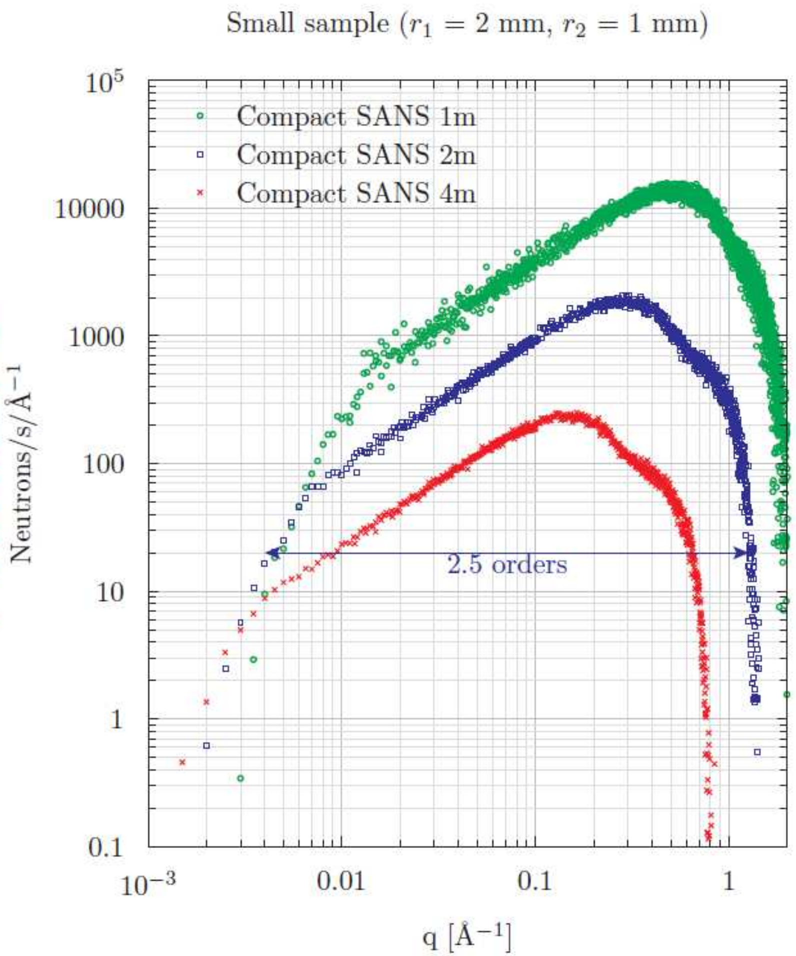


ESS

Instrument performance
Benchmark against ILL D22:

isotropic
scatterer

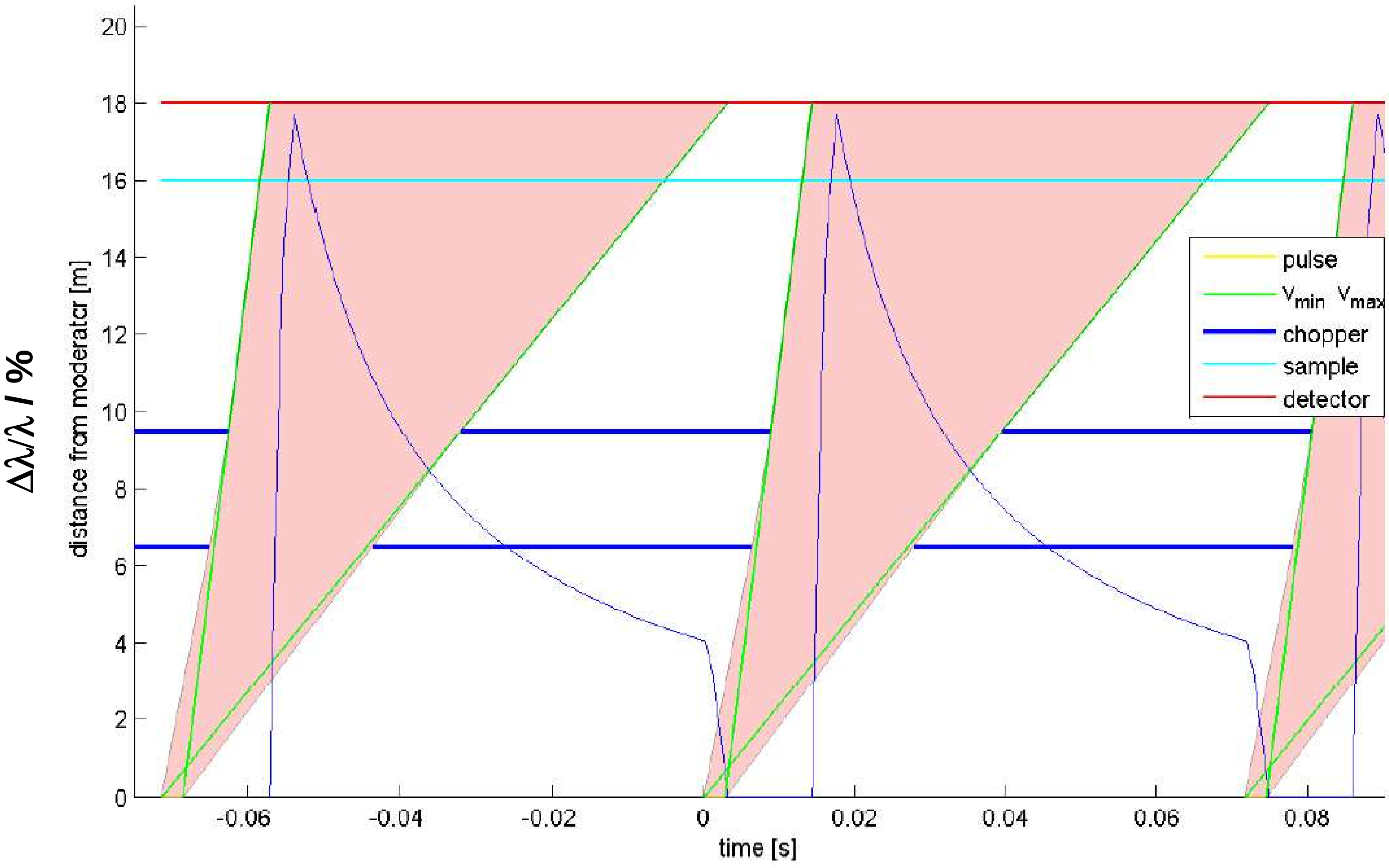




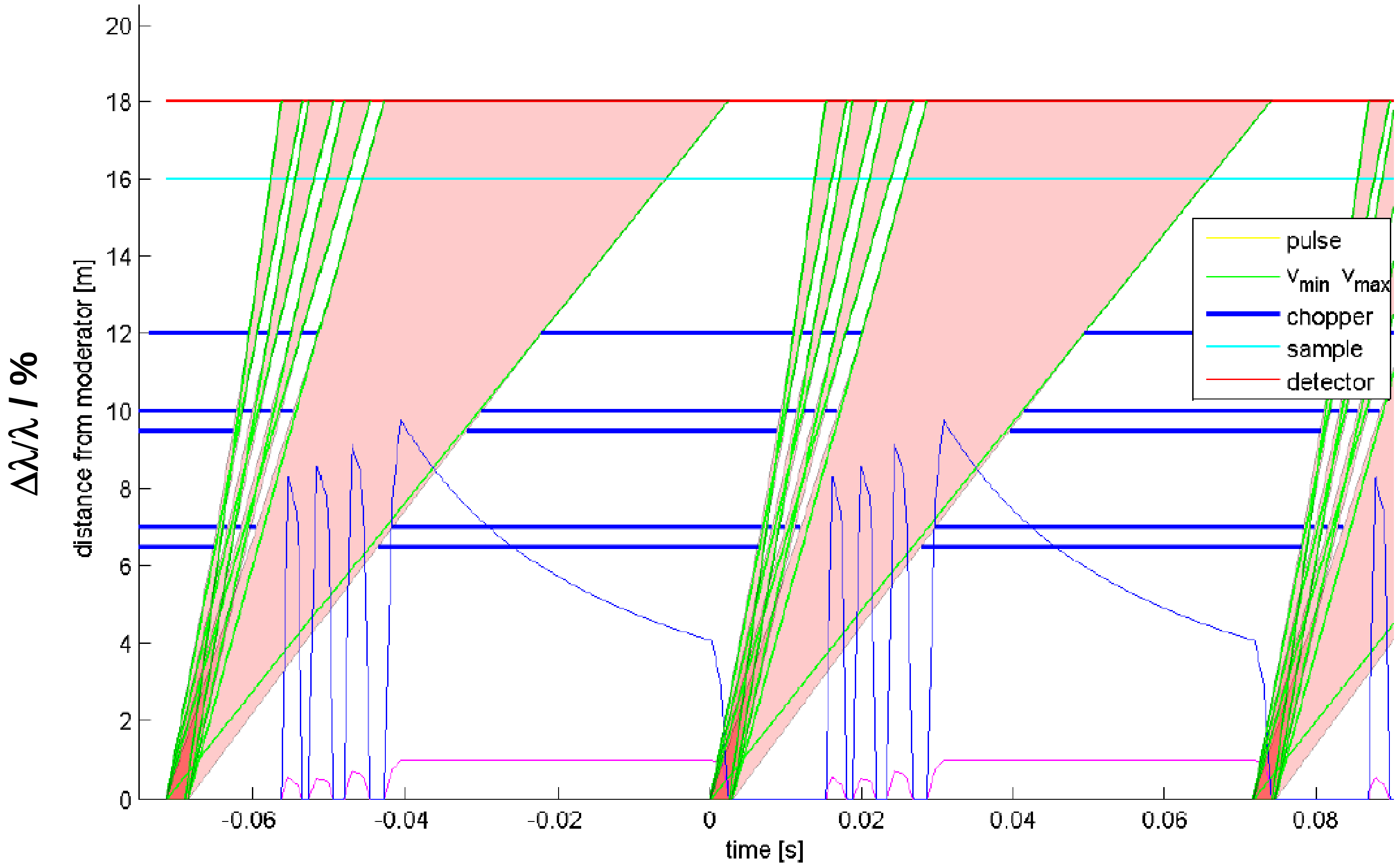
With comparable beamsizes as D22 we cover a 1.4 times wider *q*-range 20 times faster.
With small (D=2 mm^2) beam we cover a 1.4 times wider *q*-range at the same time as at ILL

ESS

Chopper setup



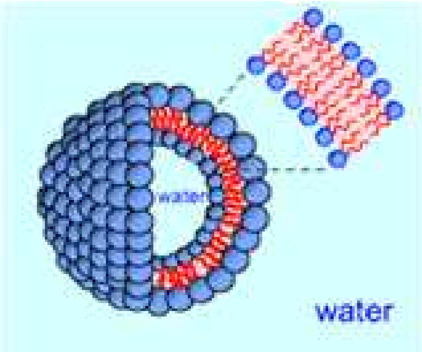
Chopper setup

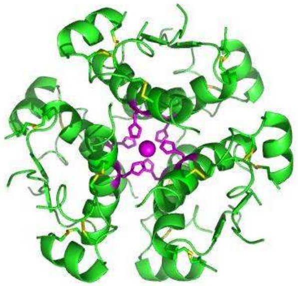


Scientific case

Main research focus:

- Bio, soft and colloidal samples in solution,
  i.e. primarily solution based samples that can be automatically handled with liquid-handling robots
- Fast time resolved experiments in a single setting broad *q*-range
- Scanning small angle neutron scattering:





***NB:** auxiliary deuteration and sample preparation facilities will be highly optimal.*

Problems/constraints:

- small sample volumes (aiming for ~10 μL at ~5 mg/ml) (2×2×2 mm^3)
- low intensity signal and small structural features

⇒*Maximize flux at the cost of wavelength resolution.*

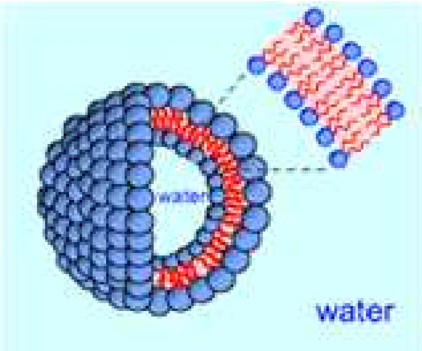
⇒*Aim for good high-q resolution.*

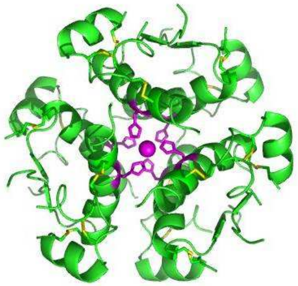
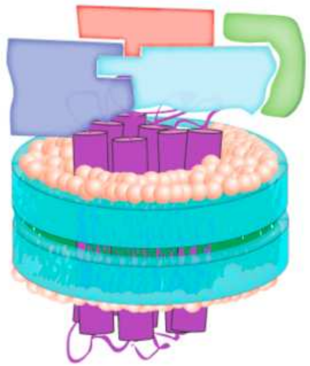
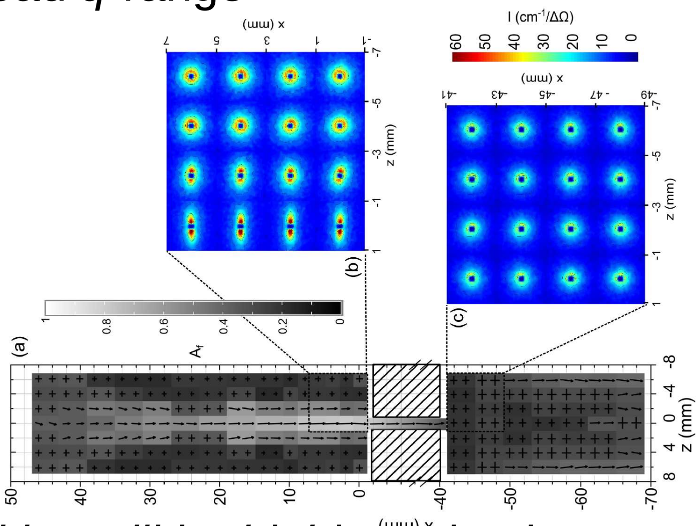
⇒*Aim for covering a very broad q-range in a single setting*

Scientific case

Main research focus:

- Bio, soft and colloidal samples in solution,
  i.e. primarily solution based samples that can be automatically handled with liquid-handling robots
- Fast time resolved experiments in a single setting broad *q*-range
- Scanning small angle neutron scattering:



***NB:** auxiliary deuteration and sample preparation facilities will be highly optimal.*

Problems/constraints:

- small sample volumes (aiming for ~10 μL at ~5 mg/ml) (2×2×2 mm^3)
- low intensity signal and small structural features

  ⇒*Maximize flux at the cost of wavelength resolution.*

  ⇒*Aim for good high-q resolution.*

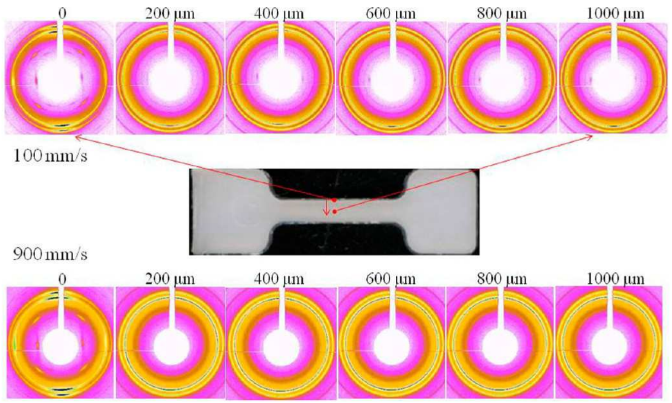
  ⇒*Aim for covering a very broad q-range in a single setting*

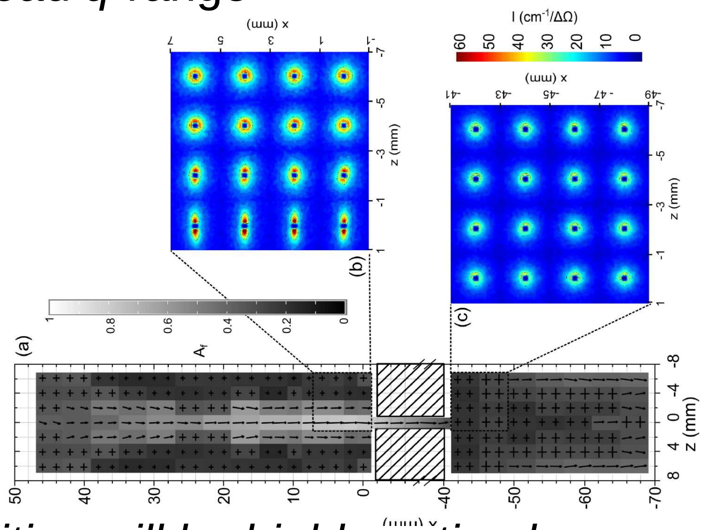
Scientific case

Main research focus:

- Bio, soft and colloidal samples in solution,
  i.e. primarily solution based samples that can be automatically handled
  with liquid-handling robots
- Fast time resolved experiments in a single setting broad *q*-range
- Scanning small angle neutron scattering:

Jiang et al.
Macromolecules, 2013,
46 (17), pp 6981–6990





***NB:** auxiliary deuteration and sample preparation facilities will be highly optimal.*

Problems/constraints:

- small sample volumes (aiming for ~10 µL at ~5 mg/ml) (2×2×2 mm^3)
- low intensity signal and small structural features

⇒Maximize flux at the cost of wavelength resolution.

⇒Aim for good high-q resolution.

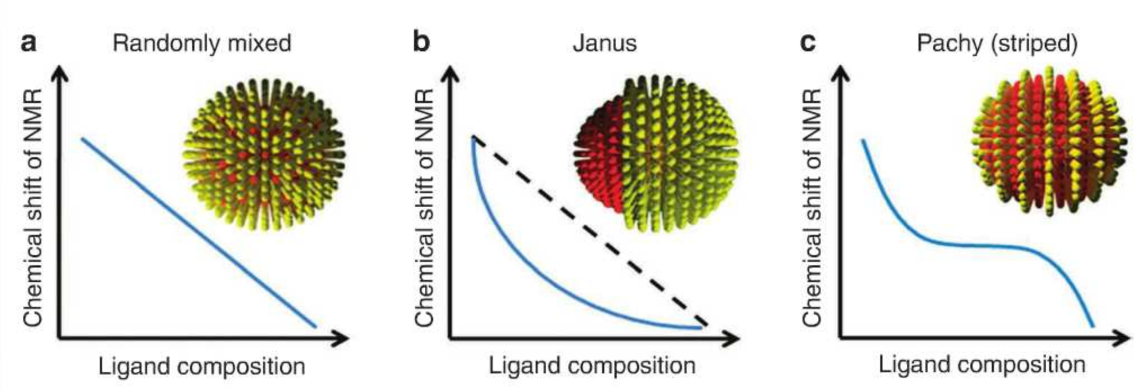
⇒Aim for covering a very broad q-range in a single setting

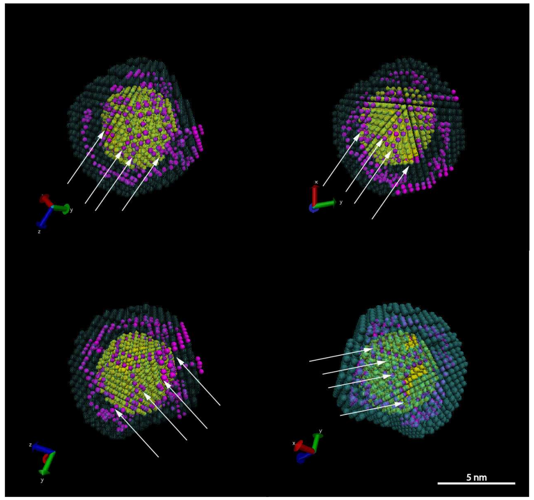
ESS

Scientific case

Main research focus:

- Bio, soft and colloidal samples in solution,
  i.e. primarily solution based samples that can be automatically handled with liquid-handling robots
- Fast time resolved experiments in a single setting broad *q*-range
- Scanning small angle neutron scattering:





***NB:** auxiliary deuteration and sample preparation facilities will be highly optimal.*

Problems/constraints:

- small sample volumes (aiming for ~10 μL at ~5 mg/ml) (2×2×2 mm³)
- low intensity signal and small structural features

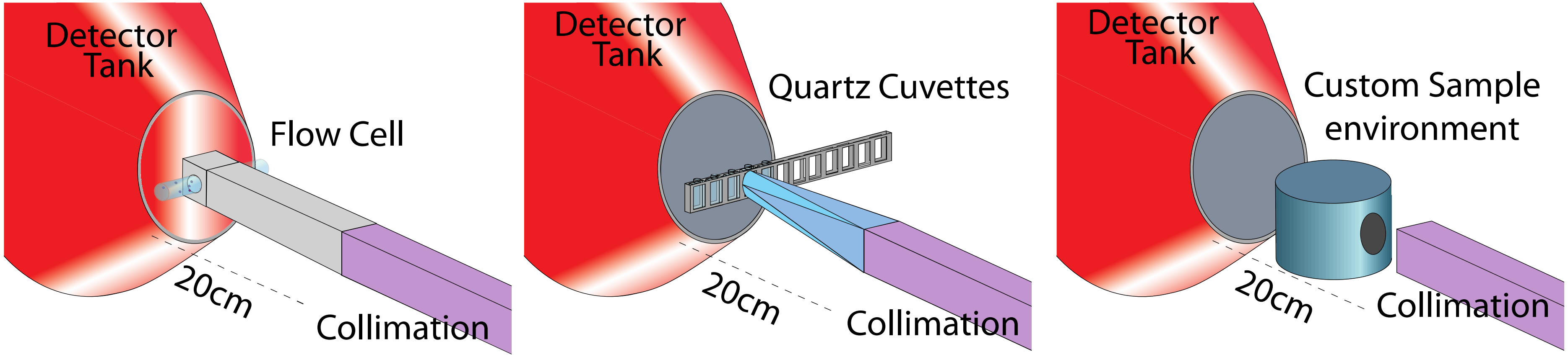
  ⇒*Maximize flux at the cost of wavelength resolution.*

  ⇒*Aim for good high-q resolution.*

  ⇒*Aim for covering a very broad q-range in a single setting*

ESS

Sample Environment

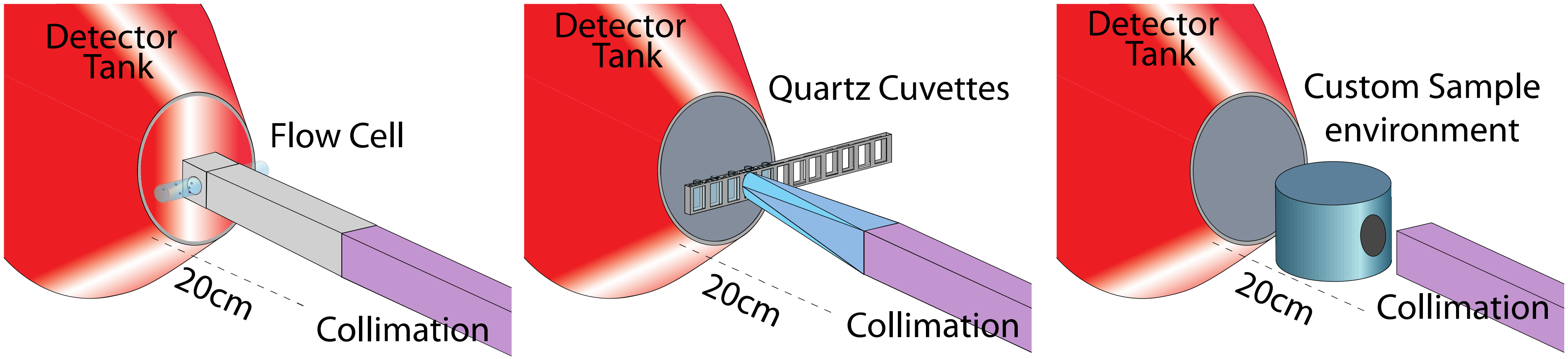


Distance from guard slit to sample kept minimal (20 cm) to allow for small beams at sample position

Sample environments that can be custom fitted into the sample space:

- Flow cell (in unbroken vacuum to minimize background)
- quartz cuvettes
- *standard rheometer*
- *pressure cell*
- *1.1 Tesla Halbach permanent magnet, 0.7 Tesla E-magnet*
- *cold finger cryostat*

Sample Environment



for bulky sample environments the detector vessel needs to be mounted on a rail system to increase the sample area.

Risk Analysis:

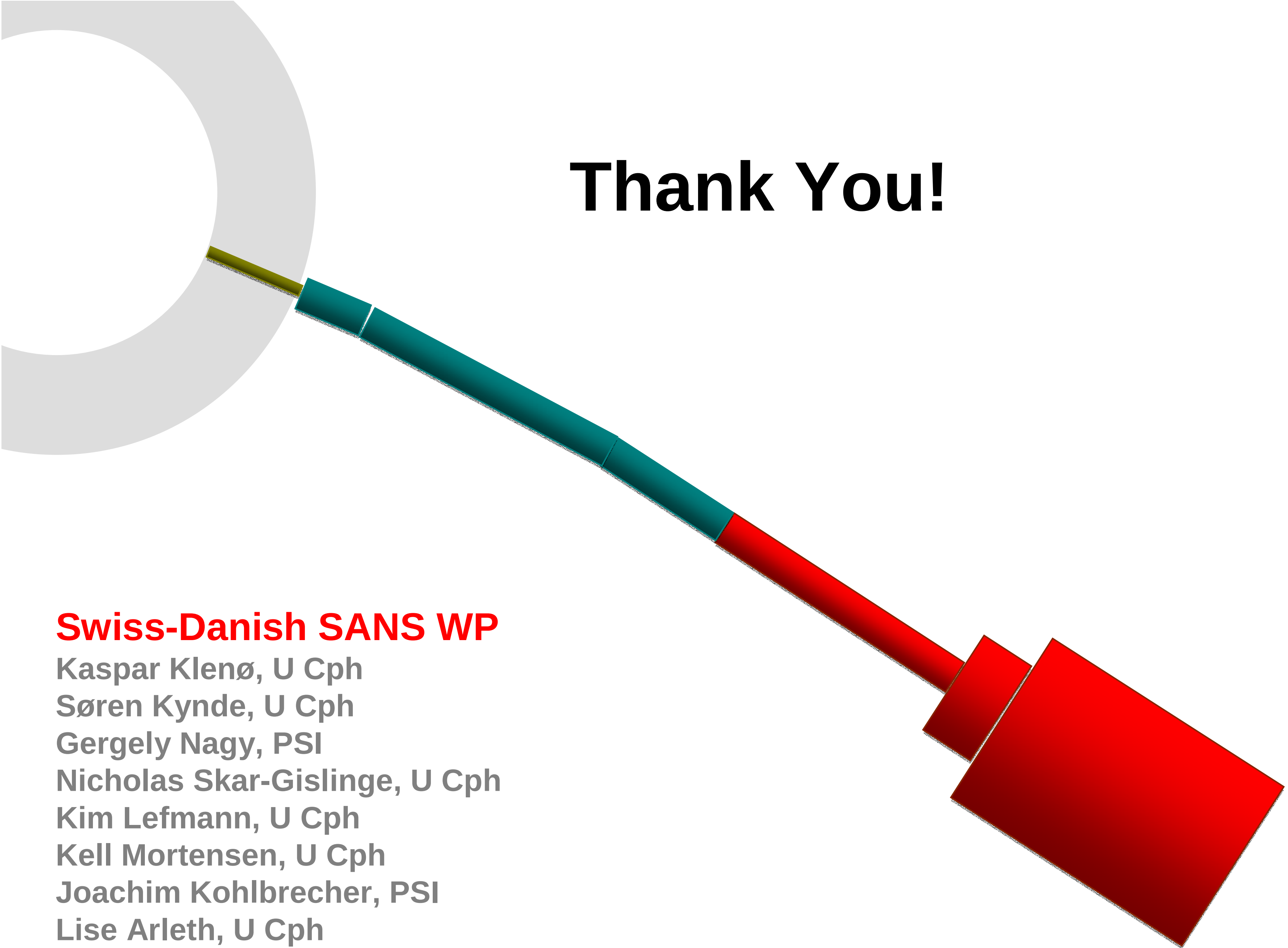
No severe technical risks are identified – But we still rely on development within Detectors, Shielding, Choppers and sample environment

Central risks:
A: That the biological user community will not become sufficiently large to use the capacity of the instrument

Mitigation:
A: Adapt the instrument for the existing soft matter community where there are heavy overload factors and where a high-flux, small sample volume instrument that covers a broad q-range in a single setting would be highly desirable and also cover new scientific territory due to improved possibilities for fast time resolved measurements and scanning SANS.

Risk of *not* dedicating a SANS instrument for the Life Sciences community: The number of SANS users from the Life Sciences community will stay at about 6% and ESS will not serve to further develop this community.

ESS



Thank You!

Swiss-Danish SANS WP

Kaspar Klenø, U Cph
Søren Kynde, U Cph
Gergely Nagy, PSI
Nicholas Skar-Gislinge, U Cph
Kim Lefmann, U Cph
Kell Mortensen, U Cph
Joachim Kohlbrecher, PSI
Lise Arleth, U Cph