DMSC-Reflectometry Workshop

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Objectives

Outline & agree the core requirements* for:

1. instrument control
2. data reduction
3. data analysis

Provide a realistic time line into full operations

Define critical dates for delivery

*core requirements are provided within the DMSC budget for construction, more with operations funding beginning in 2019.

Agenda

9:00 – 10:30 Introduction to DMSC provision and timelines

10:30-11:00 Coffee

11:00 – 12:30 Common requirements and priorities for ESS reflectometers

12:30 – 13:30 Lunch

13:30 – 14:30 Instrument-specific requirements and timelines

14:30 – 15:30 Discussion of priorities and scope

15:30 – 16:00 Summary and meeting close

Common requirements and priorities for ESS reflectometers

As far as possible everything should be the same or similar for FREIA and ESTIA

CORE REQUIREMENTS

1) instrument controls in time for cold commissioning

2) instrument SE controls, data acquisition/reduction for hot commissioning

3) instrument GUI with automatic reduction for start of user programme

(QuickNXS a good example of what should be implemented in Mantid)

ESSENTIAL FOR ESS SCIENTIFIC IMPACT

4) further development of data-analysis tools and improving the quality of the analysis by:

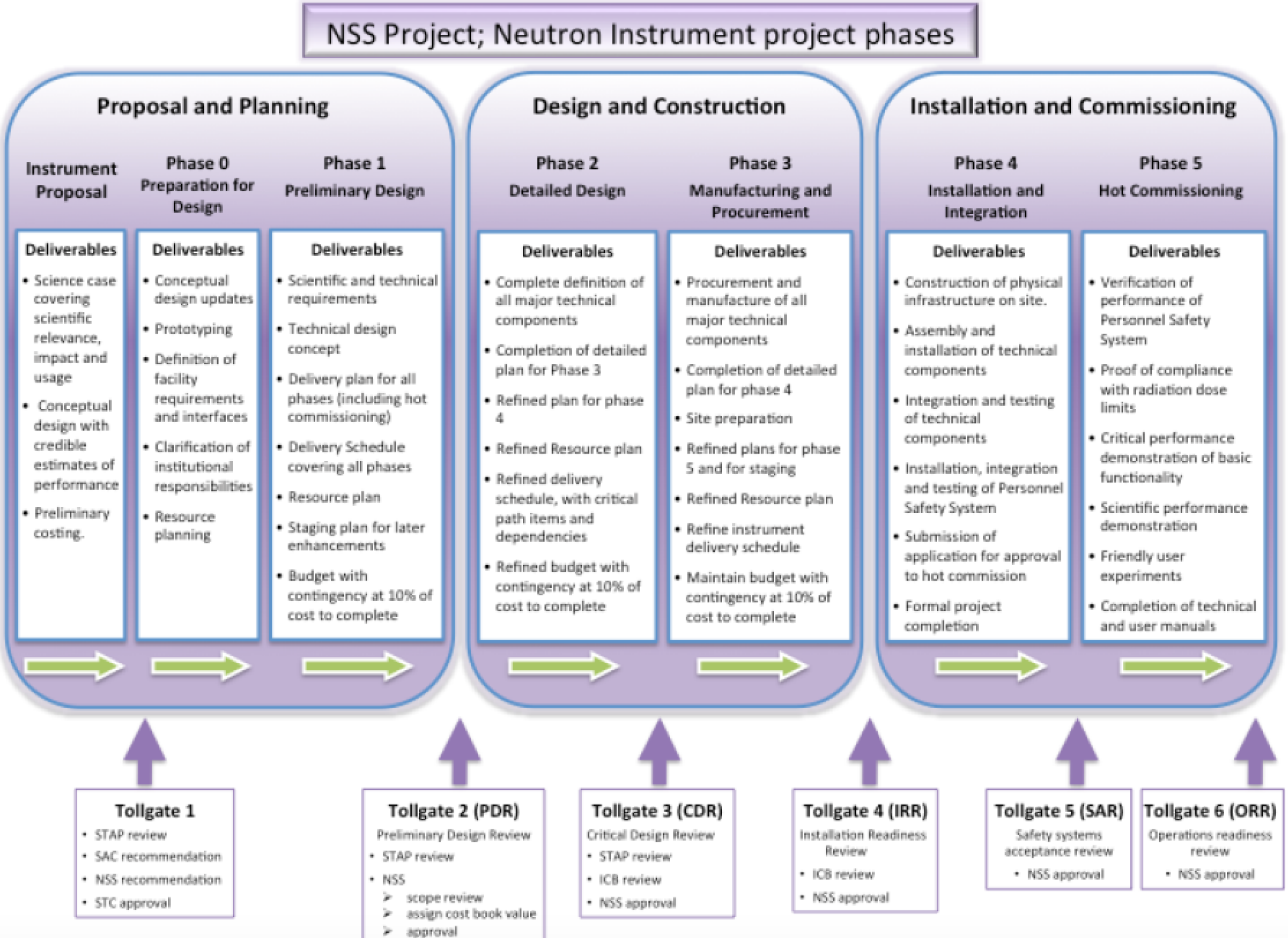
- routine tools to analyse the fits (e.g. global chi^2 maps, covariance matrices and reverse monte-carlo simulation)
- user defined input parameters and constraints (e.g. molecular volume)
- selection of different types of models (box, gaussian, b-spline, slicing pdb-structures etc.)
- analysis/fitting/modeling of backgrounds
- modeling off-specular scattering
- Linking analysis to MD simulations

ESSENTIAL FOR UPGRADES

5) GISANS analysis (not in scope of either FREIA or ESTIA)

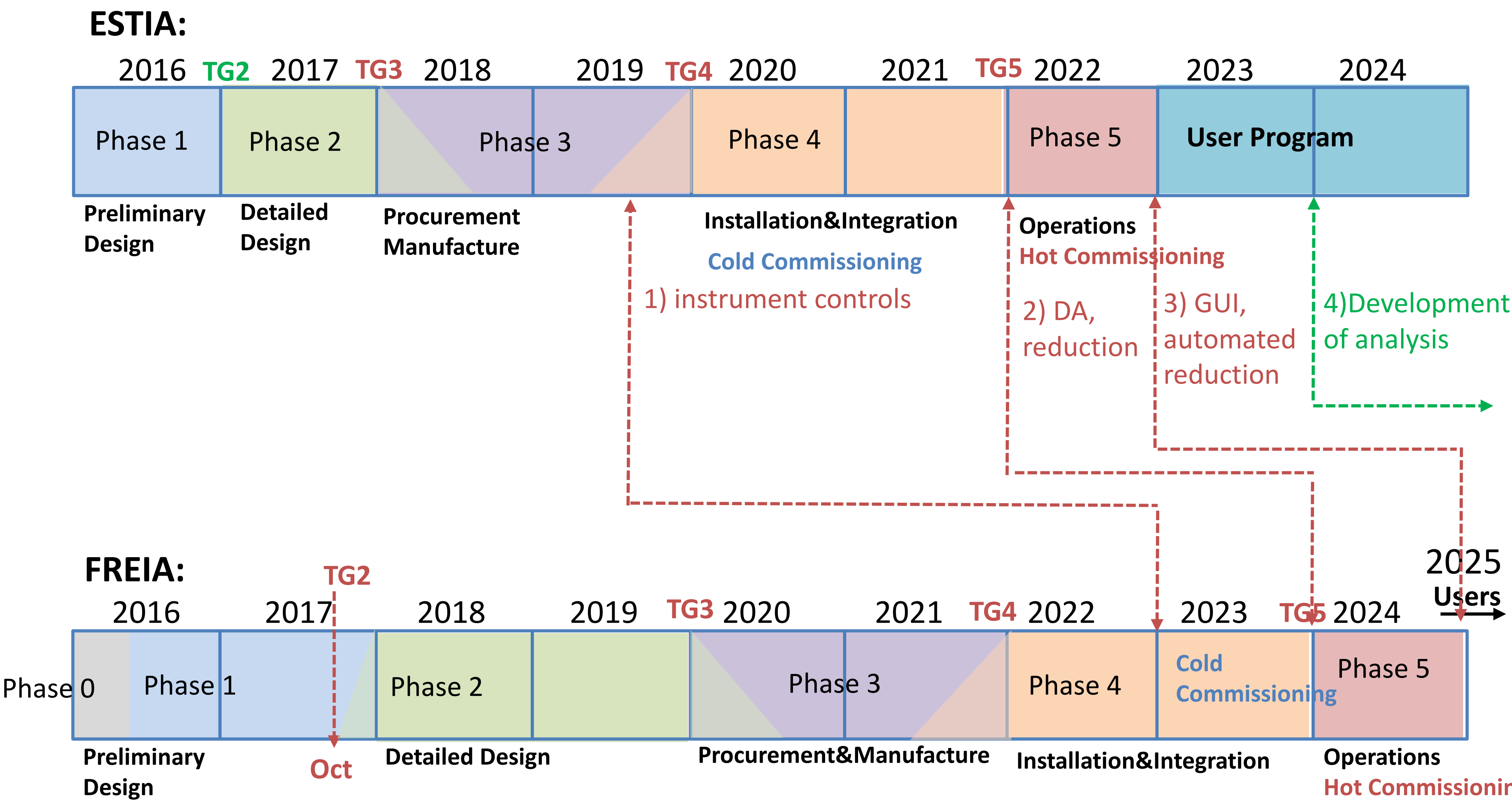
- requires development

ESS project phases



Timelines

driven by ESTIA with subsequent implementation/modification for FREIA



Common core requirements

1) instrument controls in time for cold commissioning

- *control and integration for testing during pre-build and after installation at ESS*
- data-acquisition/visualisation for detector tests (source) before neutrons

2) instrument SE controls, data acquisition/reduction for hot commissioning

- scripting interface with instrument controls, relevant alignment/calculation etc. tools, data visualisation, normalisation and manual reduction.
- Common SE controls: water baths (also ESS pool), electromagnet (pool), HPLC and syringe pumps, (laser alingment tools?)
- Instrument specific SE: several different kinds that need to be integrated and tested before user programme starts.

3) instrument GUI with automatic reduction for start of user programme

- *QuickNXS a good example of what should be implemented in Mantid*

Common analysis requirements

Requirements similar for both instruments but should be implemented for

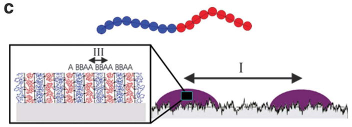
- simultaneous fitting of multiple contrast data including different solvents, polarisations or sources (neutron and X-rays)
- facile batch-loading/fitting/saving for highg data-volumes/rates
- a range of existing packages available to users but none with central facility support

-> ultimately need to develop ESS and community supported package similar to SASView.

4) further development of data-analysis tools and improving the quality of the analysis by:

- routine tools to analyse the fits (e.g. global chi^2 maps, covariance matrices and reverse monte-carlo simulation)
- user defined input parameters and constraints (e.g. molecular volume)
- selection of different types of models (box, gaussian, b-spline, slicing pdb-structures etc.)
- analysis/fitting/modeling of backgrounds
- modeling off-specular scattering
- Linking analysis to MD simulations

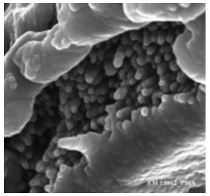
5) GISANS analysis: also for multiple contrasts, polarisations, X-ray/neutron co-refinement

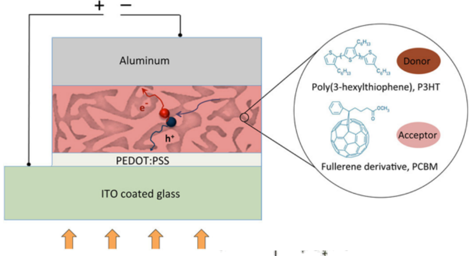


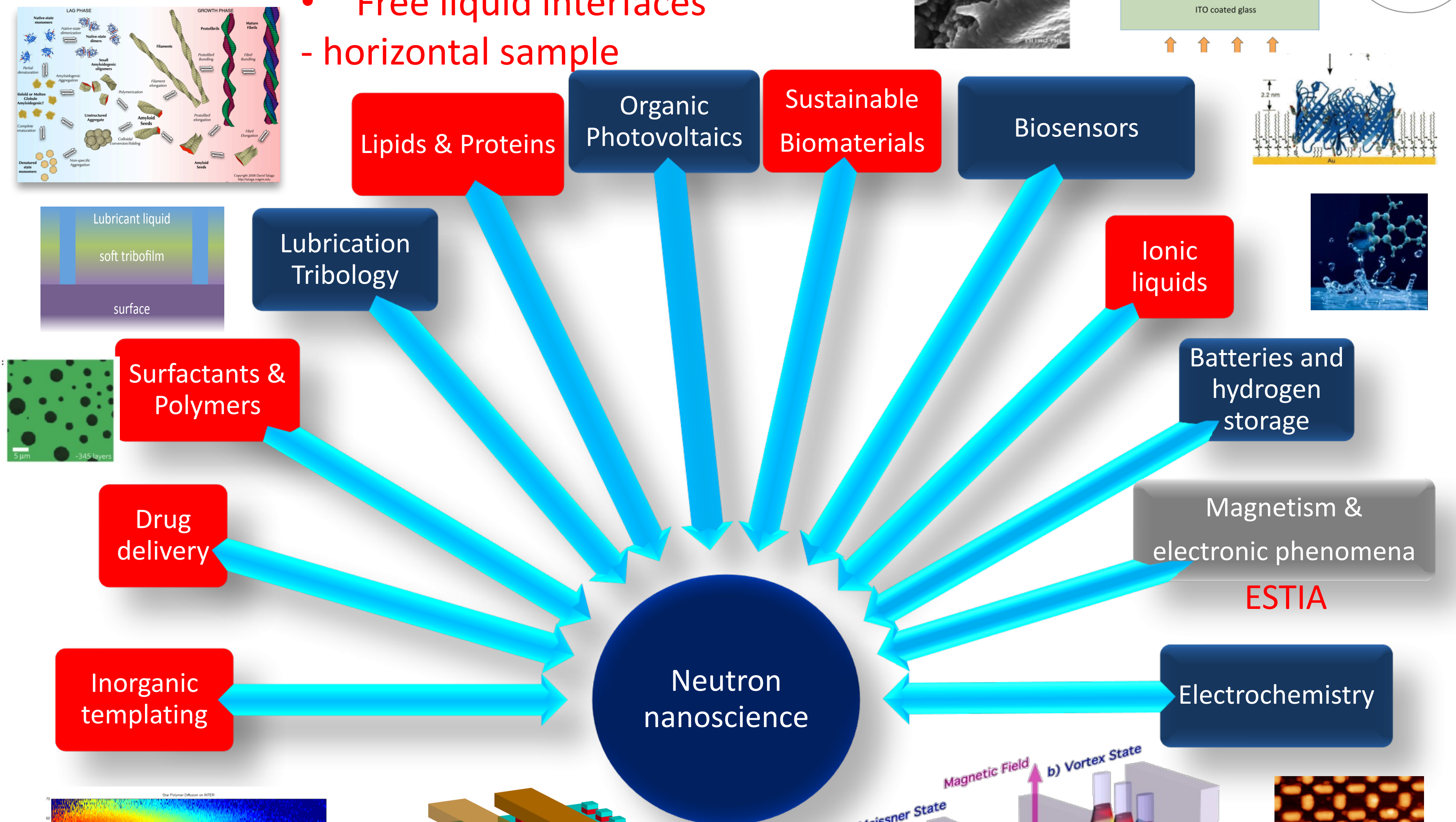
FREIA Science Case

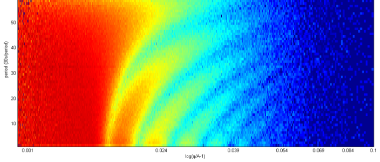
- Free liquid interfaces

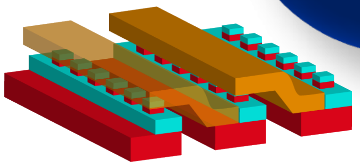
- horizontal sample

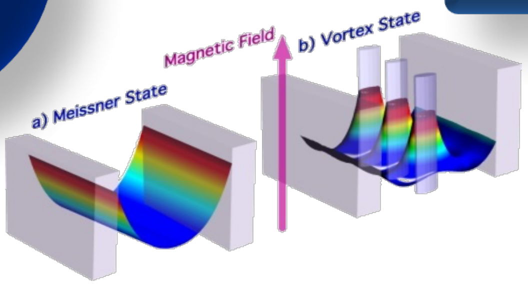


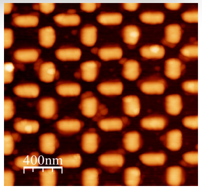




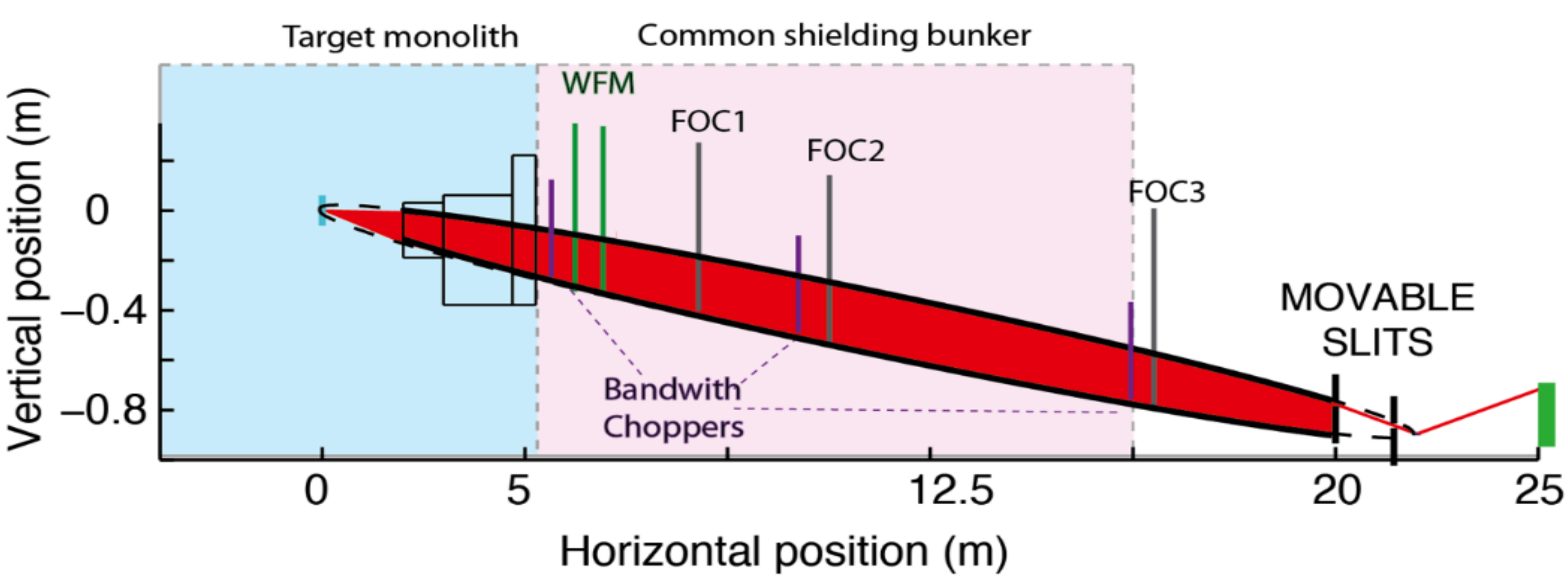




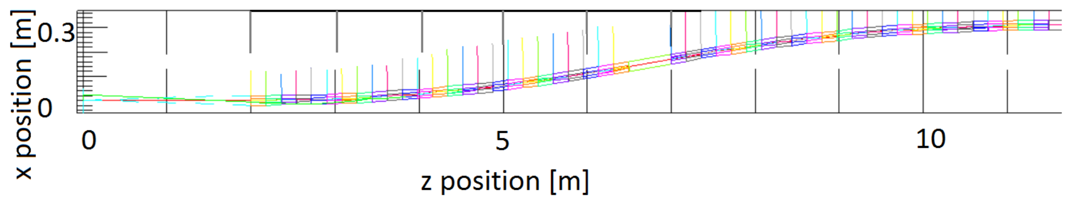




Freia Optics



- Inclined elliptical guide focuses large vertical divergence on horizontal sample surface.
- 4cm guide width horizontally
- Horizontal S-bender to avoid view of moderator



FREIA Solution

Inclined elliptical guide focuses large vertical divergence on horizontal sample surface:

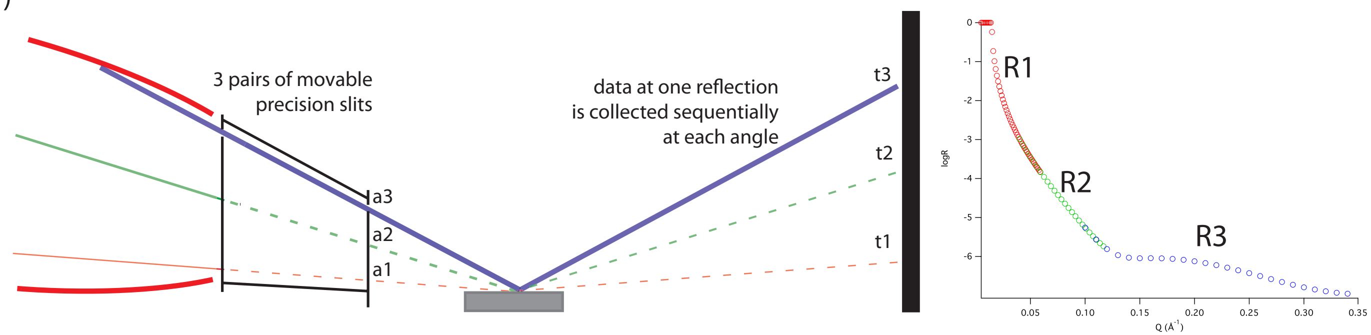
<u>Configuration/angle changes to record full Q-range often take several minutes for liquids</u>

Today: record time-resolved data at one angle with limited Q-range.

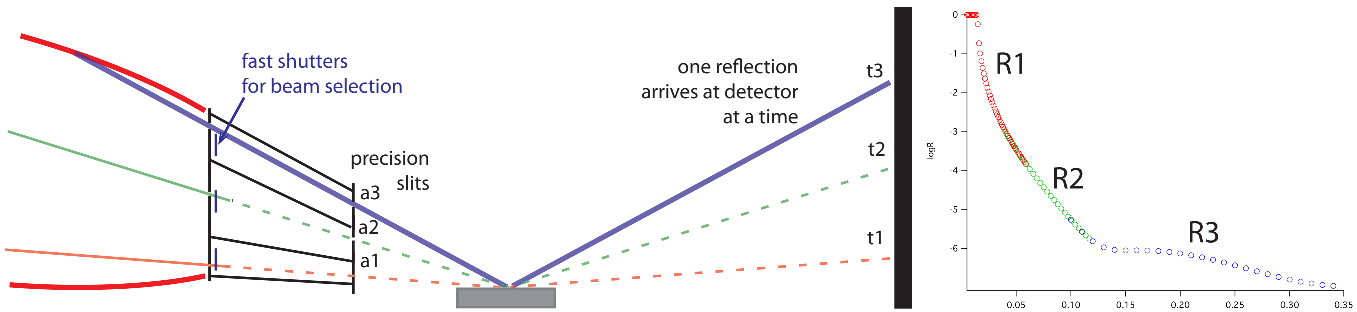
<u>At ESS, it will be possible to measure a reflectivity curve in 1-2s</u>

-> need to change angles/samples fast – avoid as many movements as possible

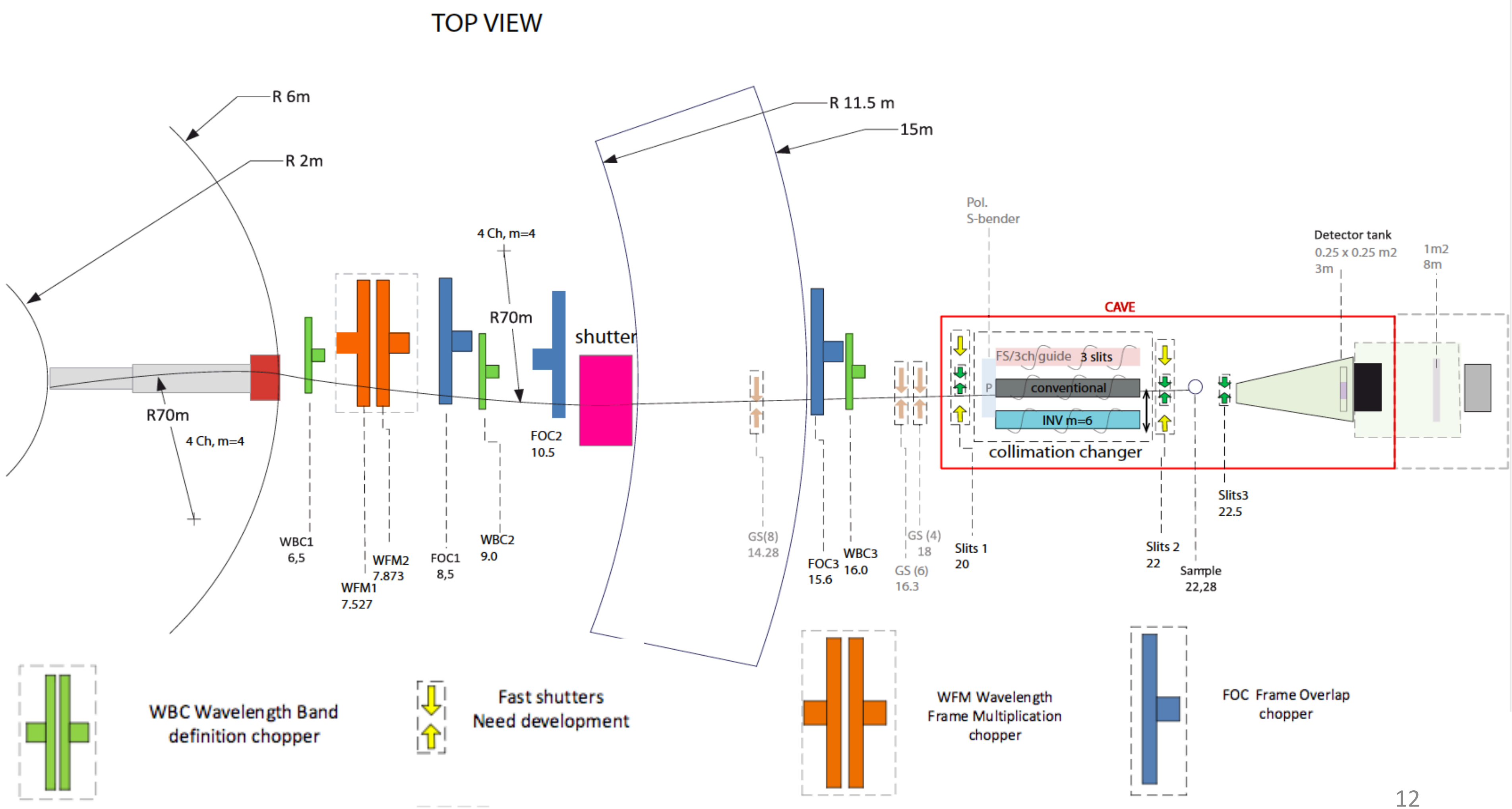
1)



2)



Freia Layout and components



Collimation options and changer

EUROPEAN SPALLATION SOURCE

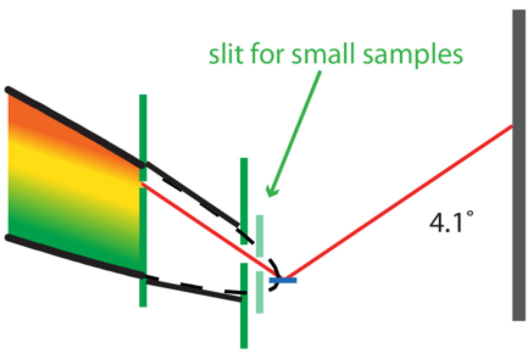
- Interchangeable 2m guide sections (20-22m from source) for :

a) conventional slit collimation

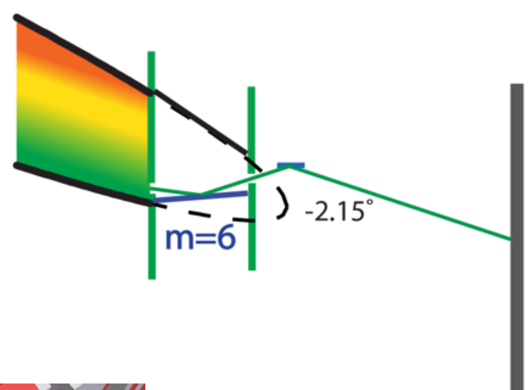
b) deflection mirror for inverted geometry (liquid-liquid interfaces, sample environments)

c) three-slit collimation (+ fast shutters) for kinetics

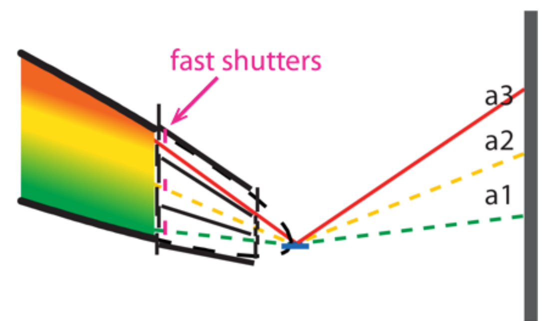
a) Conventional collimation

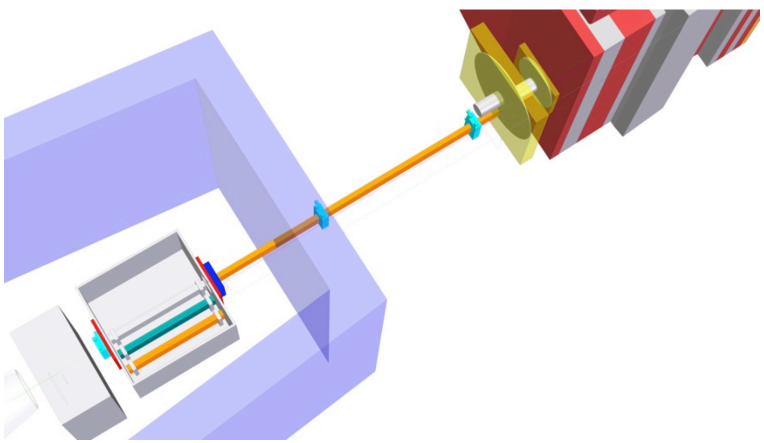


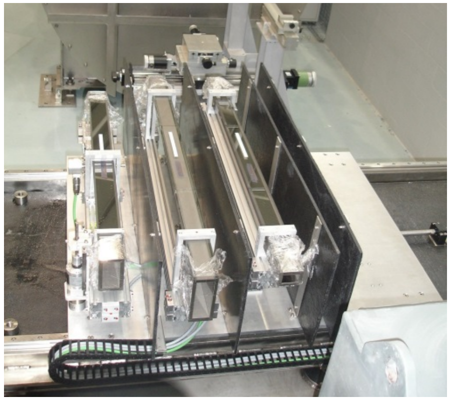
b) Inverted geometry

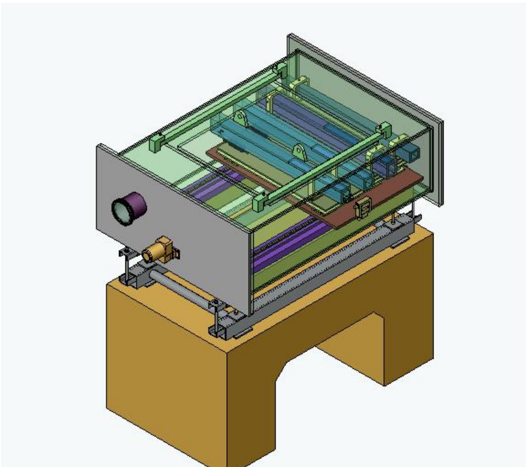


c) 3-slit collimation









e.g. collimation chamber on Platypus

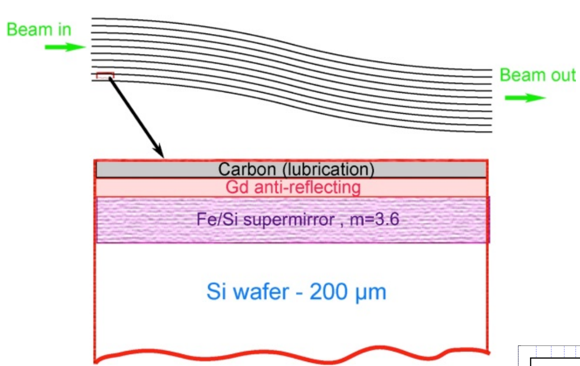
Polarisation updgrade option:

Silicon S-bender before first collimation slit for polarising beam

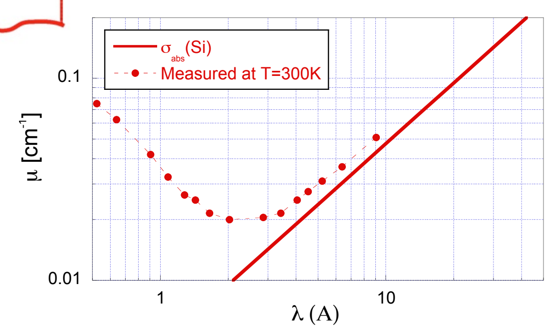
mainly for magnetic contrast films

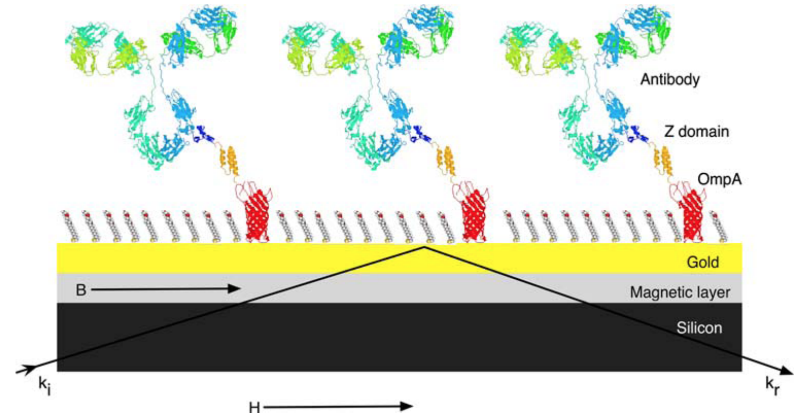
(not PA)

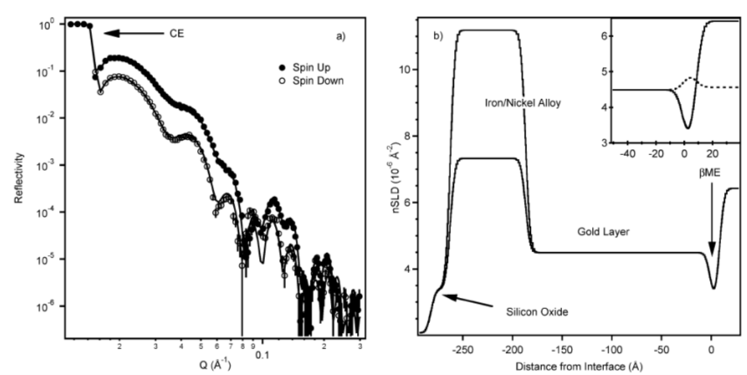
Needed for sample in which solvent contrast changes are not possible, e.g. weakly-bound antibodies in biosensor arrays.



Broad polarised wavelength band needed for kinetic PNR experiments possible at ESS.







Krist, Th., Peters, J., Shimizu, H.M., Suzuki, J., Oku, T., Physica B 356 (2005), 197-200.

Sample area and sample environments

lots of different things!

- sample stack up to at least 750kg
- coarse height-stage ± 100mm – smaller stage ± 10mm
- Two goniometers
- translation table 500mm
- gas manifold
- kinematic mounting
- laser for aligning solid samples
- laser interferometer for aligning liquids
- shielding to minimize sample background
- liquid handling manifolds (HPLC, baths)

INTEGRATION and COMMISSIONING of SE before user program can start.

ALL SE items require some degree of customisation or need to be designed in-house.

SAMPLE ENVIRONMENTS: **From Operations**

a) air-liquid adsorption troughs
b) Langmuir trough
c) set of solid-liquid flow cells
d) set of liquid-liquid cells
e) HPLC pump + syringe pump
f) water bath
g) overflowing cylinder
h) electrochemical cells

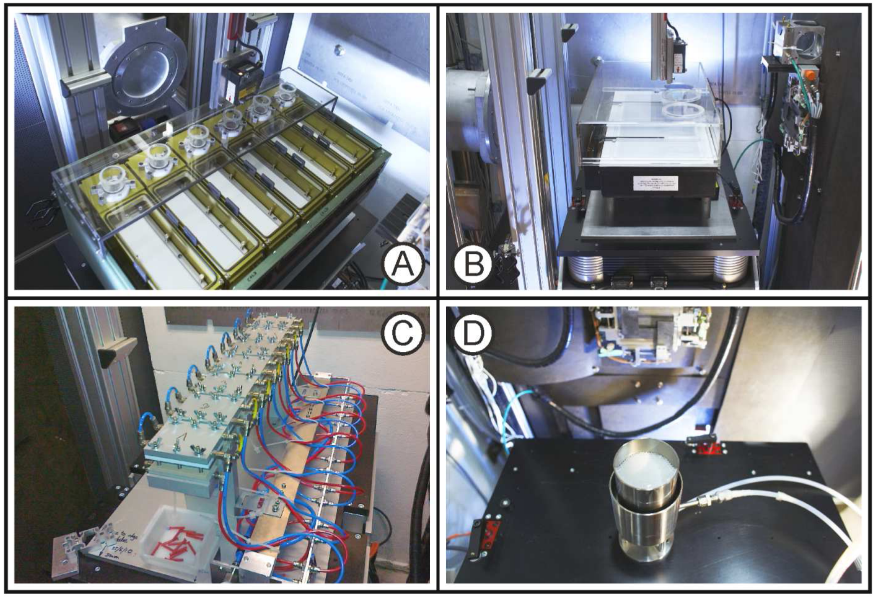
From ESS SE pool:

a) humidity chamber
b) electromagnet
c) basic vacuum chamber
d) furnace
e) rheometer
f) potentiostat (to be shared with ESTIA)

Sample changes

2-10s per sample = 1 minute per 6 samples!!!

- **Cleaning and reassembling sample cells takes 15-20 min. each time**
- *Need multiple sets of for user program*
- Large translation table for many samples
- Sample preparation area at instrument
- Lab for cleaning close by
- ***remote contrast changes (HPLC pump)***
- ***remote sample injections for kinetics (syringe pump)***



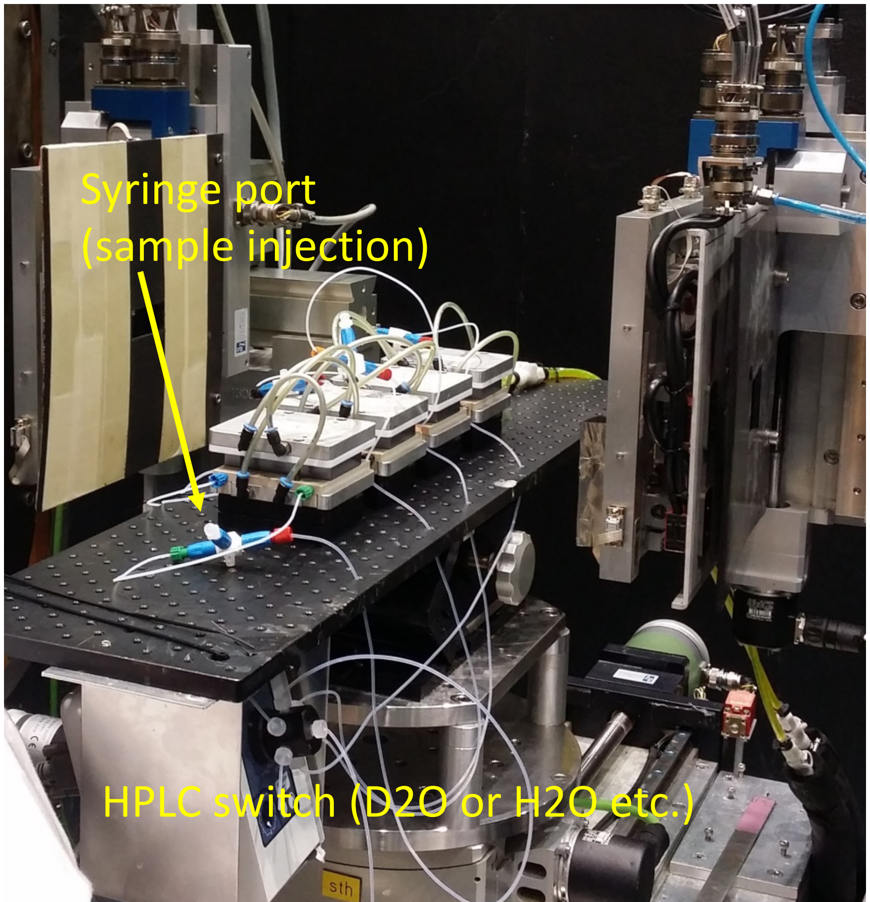
AUTOMATION WILL BE ESSENTIAL TO MACTH ESS BEAM POWER

NEED to develop robotic changers for both liquid and solid samples in the long term.

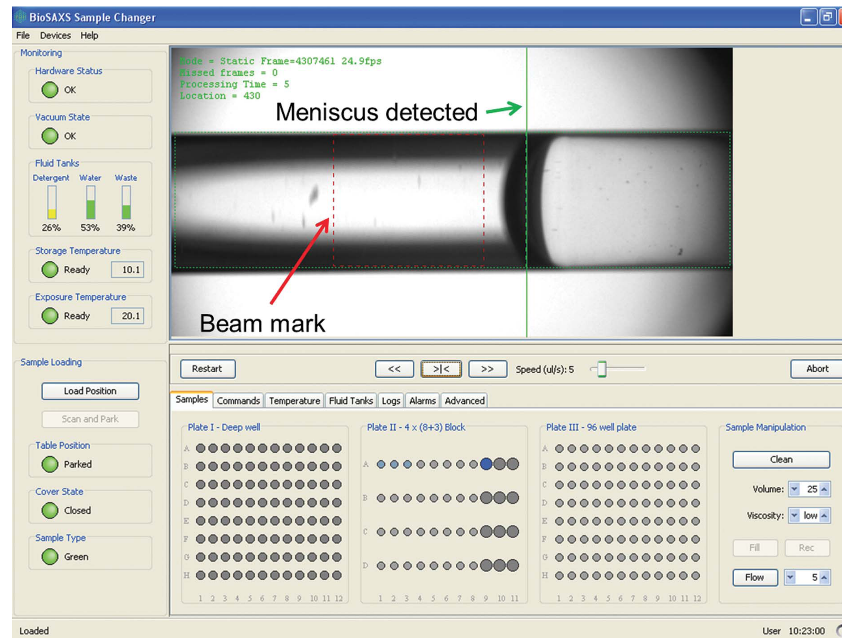
Sample changes

2-10s per sample = 1 minute per 6 air-liquid chambers!!!

- remote contrast changes (HPLC pump)



- remote sample injections for kinetics – *autosampler* – cf. BioSAXS:



AUTOMATION WILL BE ESSENTIAL TO MACTH ESS BEAM POWER

NEED to develop robotic changers for both liquid and solid samples in the long term.

Detector and housing

REF: 0.3m x 0.3m (in scope: 0.25 x 0.25cm) area detector at 3m from sample in a tank (Argon)

- > measure Q = $1Å^{-1}$ (11.5 °) on solid samples (#2)

Most liquid measurements within 0.25°- 4.1° without moving detector (#1)

Movement range for inverted beam geometry

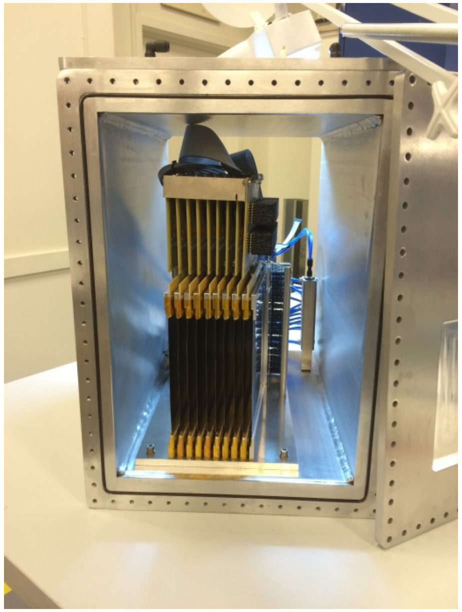
GISANS Upgrade: $1m^2$ area detector at 8 m from sample position in evacuated tank

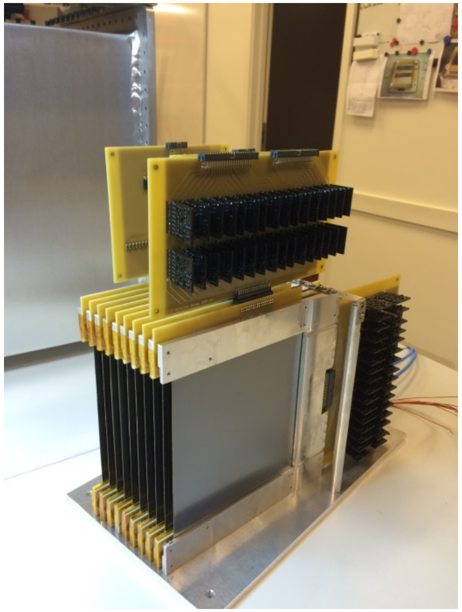
GISANS detector position and size are determined by the required Q_y range (3×10^{-3}- 0.25 $Å^{-1}$)

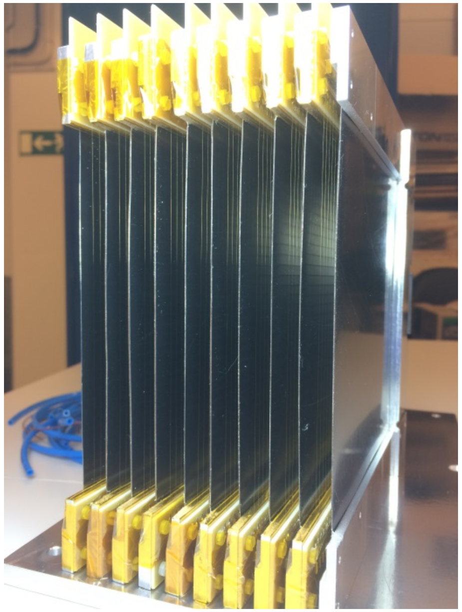
Based on ^{10}B Multiblade detector developed at ESS (Francesco Piscitelli)

Cylindrical arrangement of blades -> fixed detector distance, radial vertical translation

Resolution requirements: 0.5mm vertically and 2.5mm horizontally.







FREIA specific requirements

Instrument controls:

- laser interferometer for liquid height alignment with feedback loop to sample z-stage
- three-slit collimation – options for easy configuration for kinetic experiments
- 7-fold WFM choppers + 3 frame overlap choppers

SE:

- Lots of various sample changers – easy options for configuring no. of angles/runs/metadata
- Langmuir trough(s) – control of surface pressure and area with interface for calculating area per molecule from sample concentration (cf. NIMA troughs – implemented in NOMAD @ILL)
- controls for different liquid pumps for changing samples – same as for ESTIA.

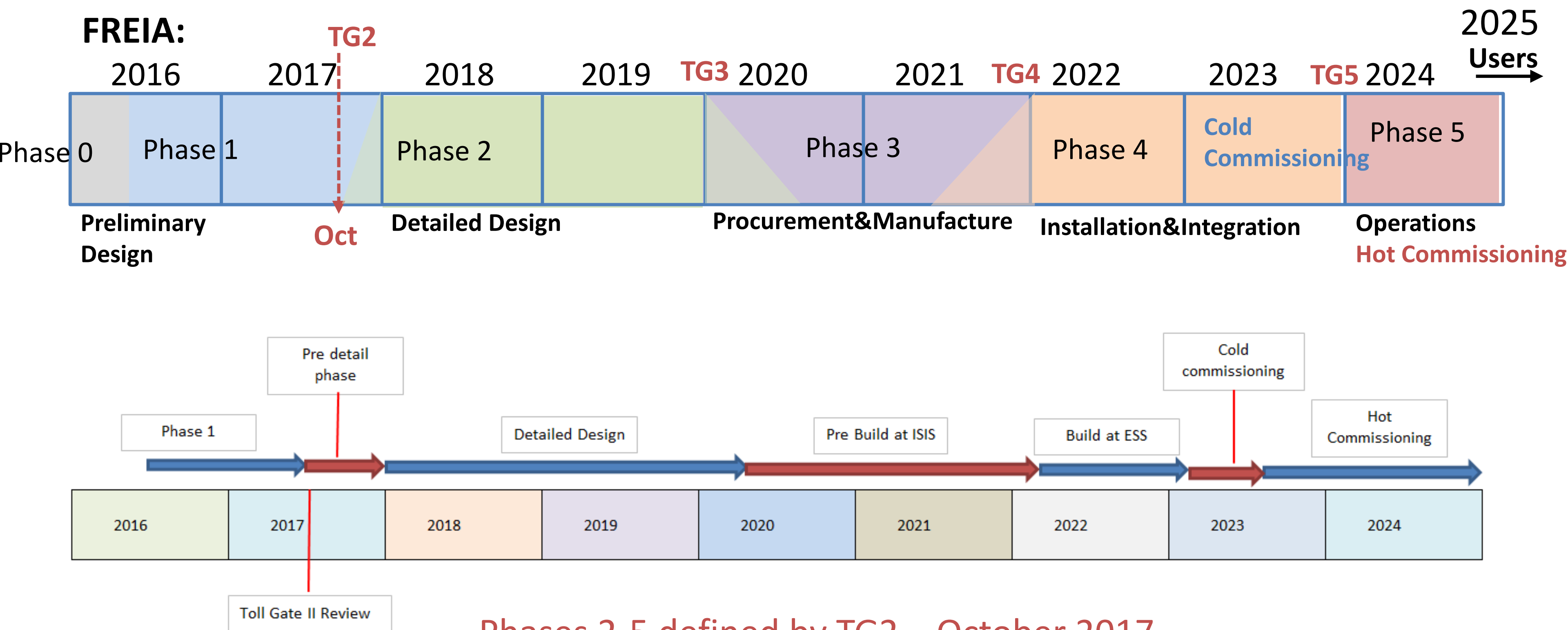
Reduction:

- reduction of 7-fold WFM data
- use of configuration and metadata for SE to autoreduce data from multiple samples
- easy background subtraction for 3-slit data
- inclusion of SE data (e.g. Langmuir trough readout) – partly implemented on Inter @ ISIS

Analysis:

- fitting several angles with different/variable resolution (also for ESTIA)

FREIA timeline



Phases 2-5 defined by TG2 – October 2017
-> start of cold commissioning/controls needed
for pre-build at ISIS in any case later than 2019.

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March 2017