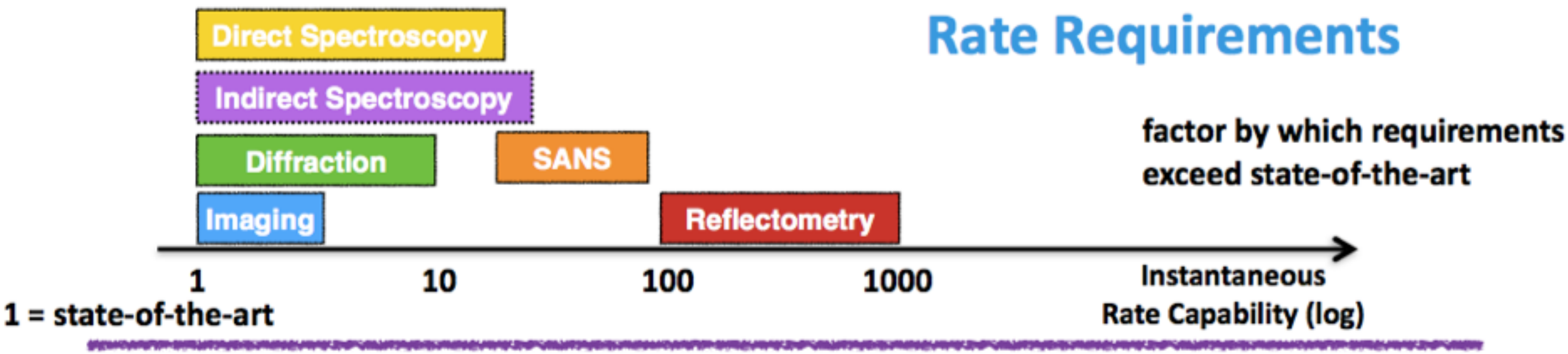
Outline

- What Challenges does ESS present for
  - Data Reduction and visualisation
  - Experiment control
- What is Instrument data delivering
    - Core frameworks that fit into ESS architecture
    - Specific technique and instrument customisations
- What relevance our scope has to commissioning.

Data rate challenge



The detector rate challenge presents the same challenge to DMSC

Integrated controls and Timing

EUROPEAN SPALLATION SOURCE

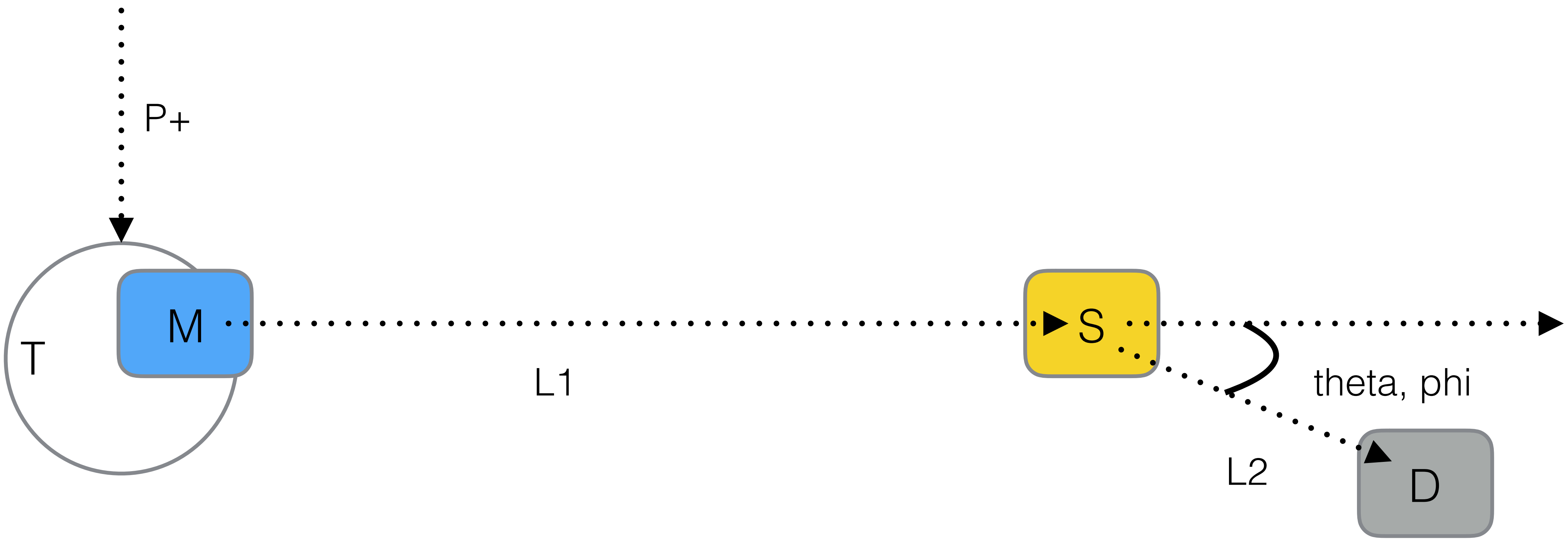
- Distributed timing system

- ICS deliver key services to Machine and Science

Data reduction

- Data reduction is
  - Transforming the data from the instrument coordinate system to the science coordinate system.
  - Correcting the data for instrumental and source artefacts
  - Correcting the data for absorption and multiple scattering

Data reduction



- Convert T.O.F to energy, wavelength, momentum transfer, d-space.
- Precise knowledge of flight paths
- Precise knowledge of scattering angle
- Geometry is essential

Data rate

- Event rates calculated from instrument proposal data
- Event data is collected as a list of timestamps for each spectrum
- High data rate creates a long list
- ESS average rate is ~8GB /min

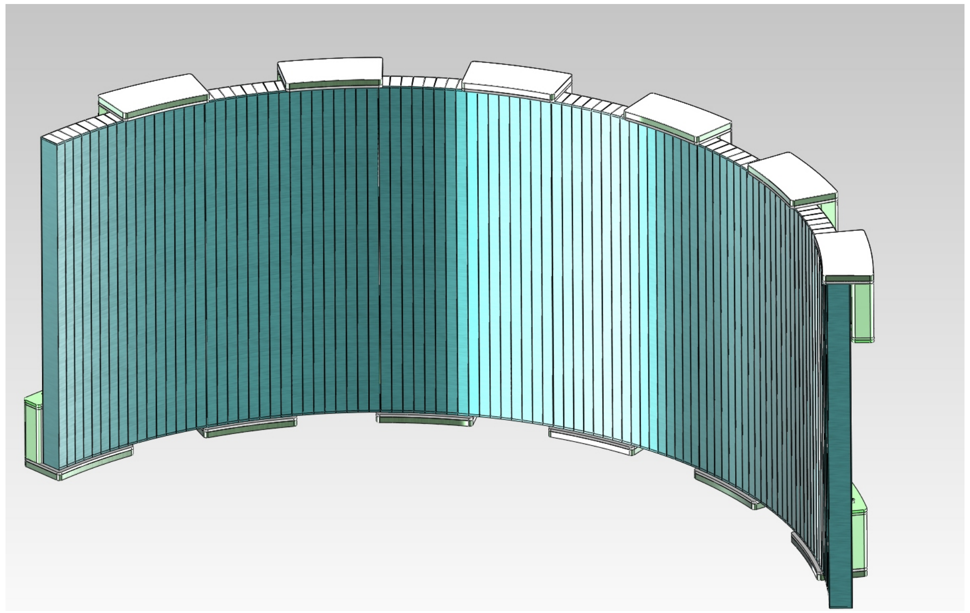
	Event rate corrected for sample scattering	MB/s/MW	1 minute collection GB (1MW)
LOKI	1.E+06	20	1.2
SKADI	0.E+00	20	1.2
Estia	4.E+07	500	30
Friea	6.E+05	10	0.6
Dream	9.E+06	100	6
Hiemdal	1.E+07	150	9
BEER	2.E+05	3	0.18
Magic	4.E+07	500	30
NMX	7.E+03	0.1	0.006
ODIN	-	150	9
CSPEC	3.E+06	40	2.4
TREX	7.E+05	10	0.6
MIRICLES	3.E+05	4	0.24
BIFROST	0.E+00	4	0.24
VESPA	3.E+05	4	0.24

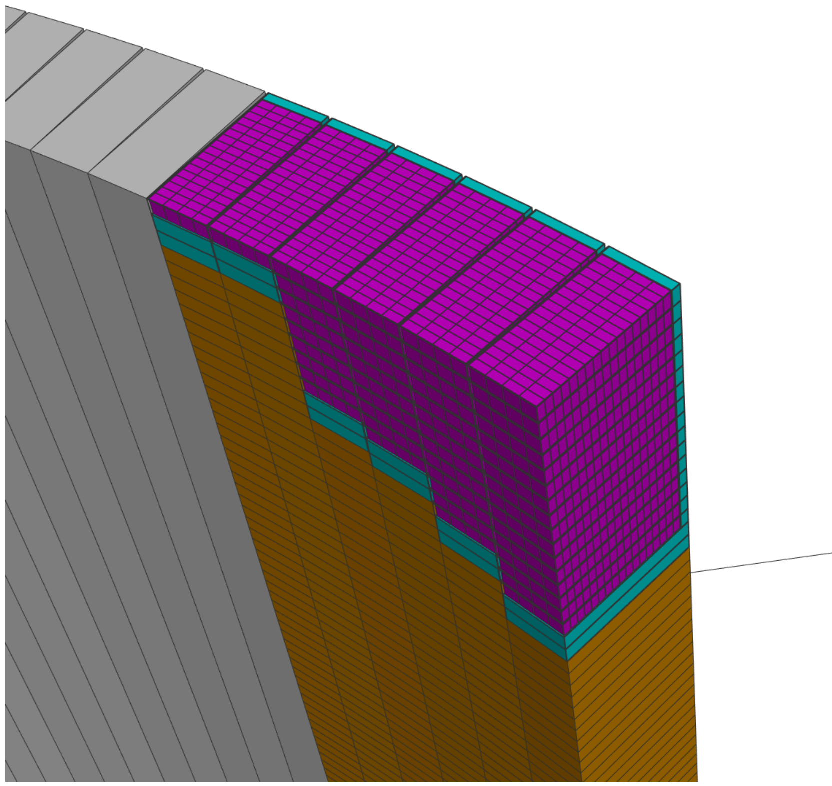
To solve the data rate challenge

- The processing has to keep up with the experiment
- Optimise software, hardware and network
- Use the ADARA method of acquisition and live data treatment.
- Use automated reduction
- Use distributed computing SAAS
- Improve Mantid performance

The detector geometry challenge

- 3 key issues
  - Shape
  - Position
  - Number



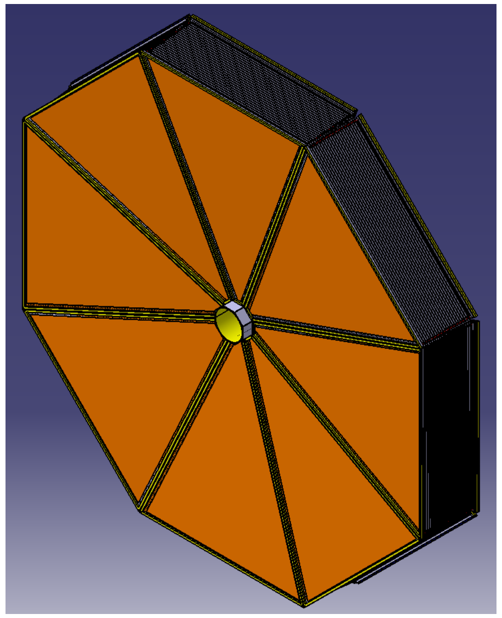


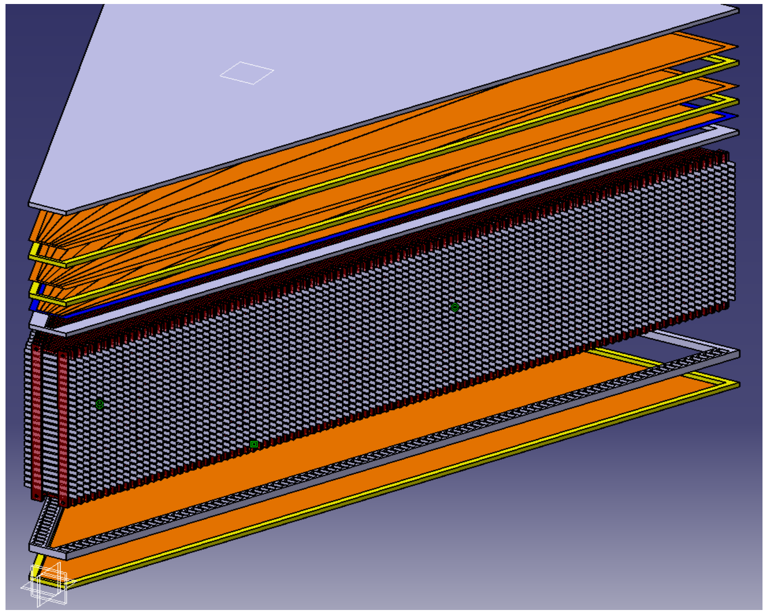
- 10B Detectors are not geometrically simple to describe

- Channel count is increased to deal with the rate

- Each instrument is different

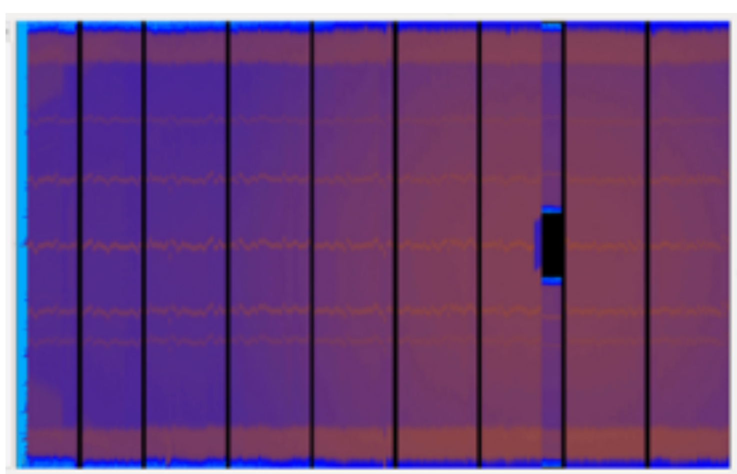
- Instrument detectors are not always static

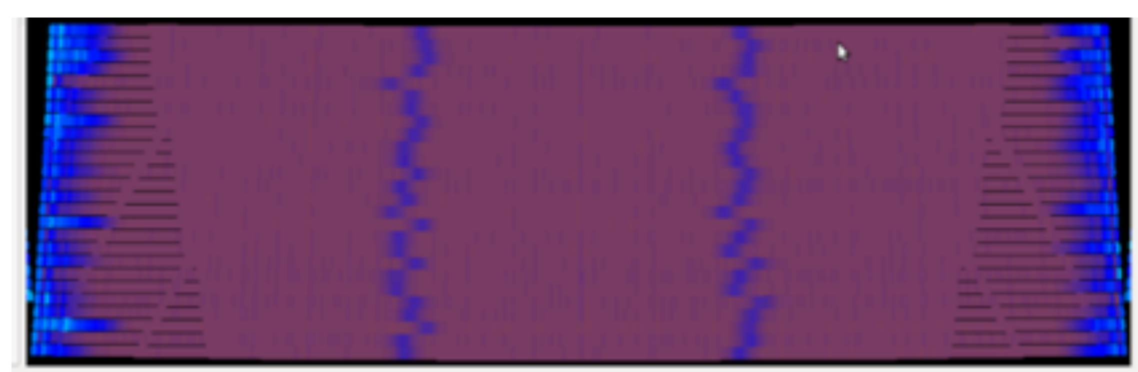




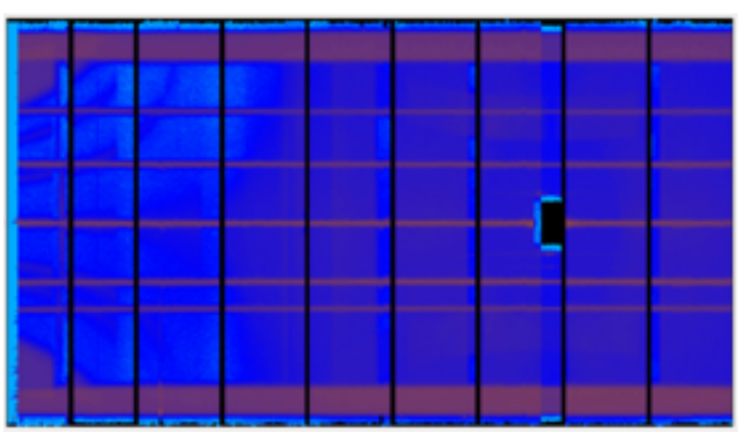
Geometry & calibration

- Scientifically the actual r,t,p and x,y,z co-ordinates are required.
- One cannot rely on the engineering positions.
- 10B Geometries add an extra dimension to this problem.
- Gas pressure is not fixed therefore gain is not fixed over time





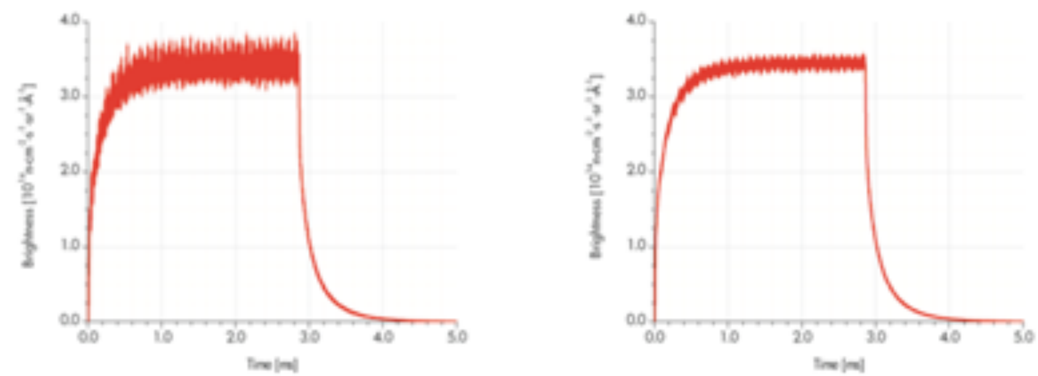
Uncalibrated PSD bank



Calibrated PSD bank

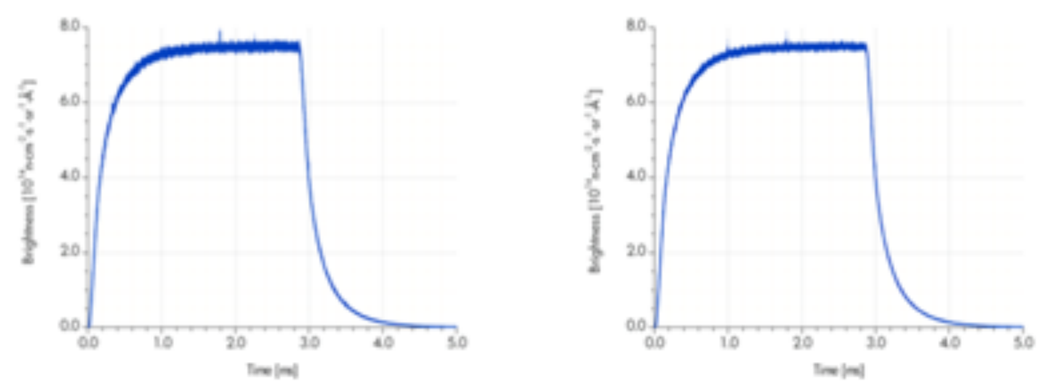
The source challenge

- There is no existing long pulse spallation neutron source.
- Fluctuations in the ion source will lead to fluctuations in neutron flux ~8%
- Proton beam rastoring will cause fluctuations ~10-20%
- WFM is new and essentially untested
- Normalisation of data will be challenging
- Stitching poorly normalised data is not possible.



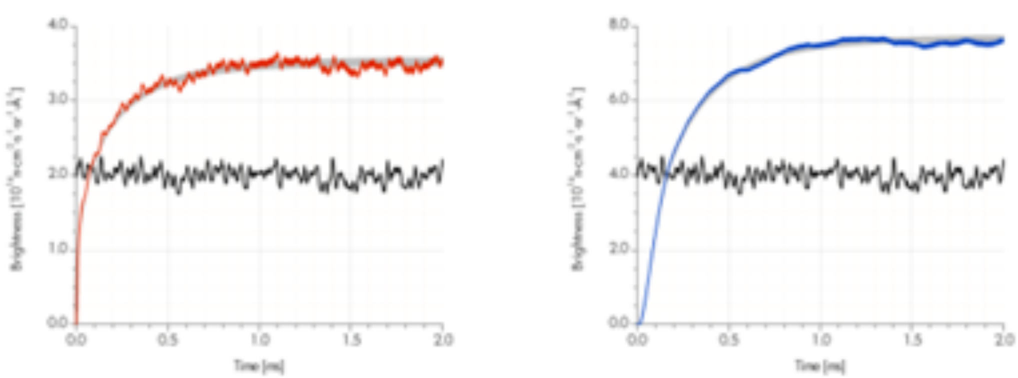
(a) 0.8 Å neutron pulse produced by thermal moderator from a single rastered pulse.

(b) 0.8 Å neutron pulse produced by thermal moderator averaged over 2 rastered pulses: direct and inverted.



(c) 2.5 Å neutron pulse produced by cold moderator from a single rastered pulse.

(d) 2.5 Å neutron pulse produced by cold moderator averaged over 2 rastered pulses: direct and inverted.



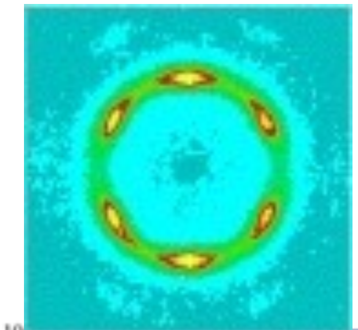
(a) 0.8 Å neutron pulse produced by thermal moderator: grey line from ideal proton pulse, red line from worst case proton pulse (black line, not to scale)

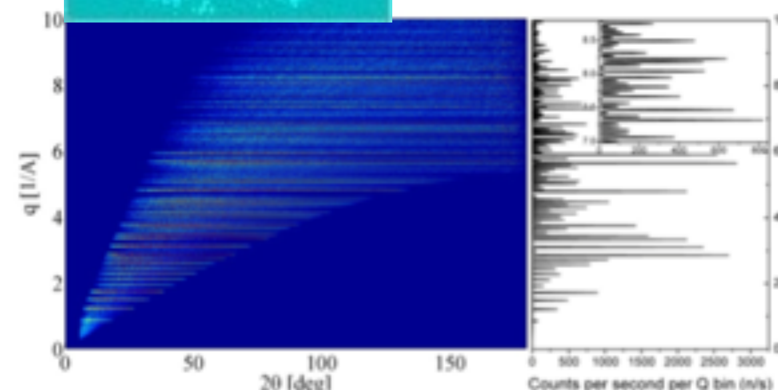
(b) 2.5 Å neutron pulse produced by cold moderator: grey line from ideal proton pulse, blue line from worst case proton pulse (black line, not to scale)

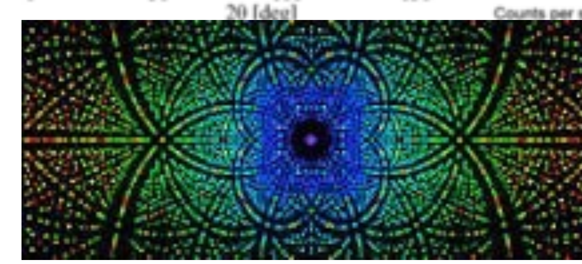
Examples for ESS

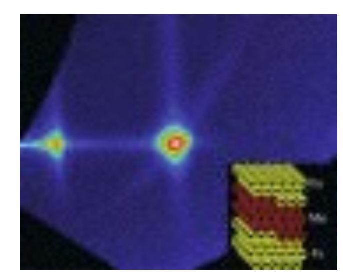
EUROPEAN SPALLATION SOURCE

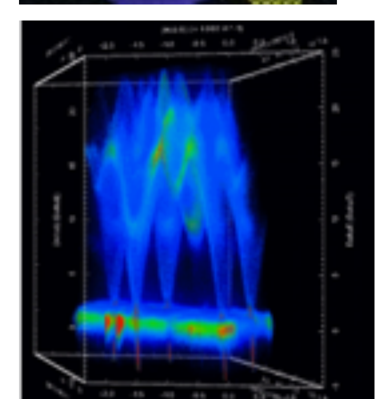
- SANS
  - Correction of data to 1D or 2D I(q) or I(qx,qy)
- Powder diffraction
  - Correction of data to 1D representation of intensity vs d spacing
- Single crystal diffraction
  - Peak finding and integration to list of HKL integrated intensity & sigma
- Reflectometry
  - Correction of data to 1D I(q) or 2D I(qx,qy)
- Spectroscopy
  - Correction to S(q,w)
  - Generation of 4D datasets











Reduction deliverables for instruments

- Massively improved Mantid core framework
- Automated reduction service*
  - Distributed architecture (MPI)
- Reduction scripts & workflows
- Interface to UI
- Integration with automated reduction
- Integration to the experiment control
  - managed configurations
  - Vanadium files
  - background data

*Mantid will run as a service to the experiment control and DAQ this allows for things such as experiment steering

Data visualisation

- Higher rates = more data
- Distributed reduction
- Remote access
  - The data is not on a local machine - its too big
- 4D data
  - Parametric studies
  - …
- Utilise distributed paraview

Deliverables for instrument commissioning

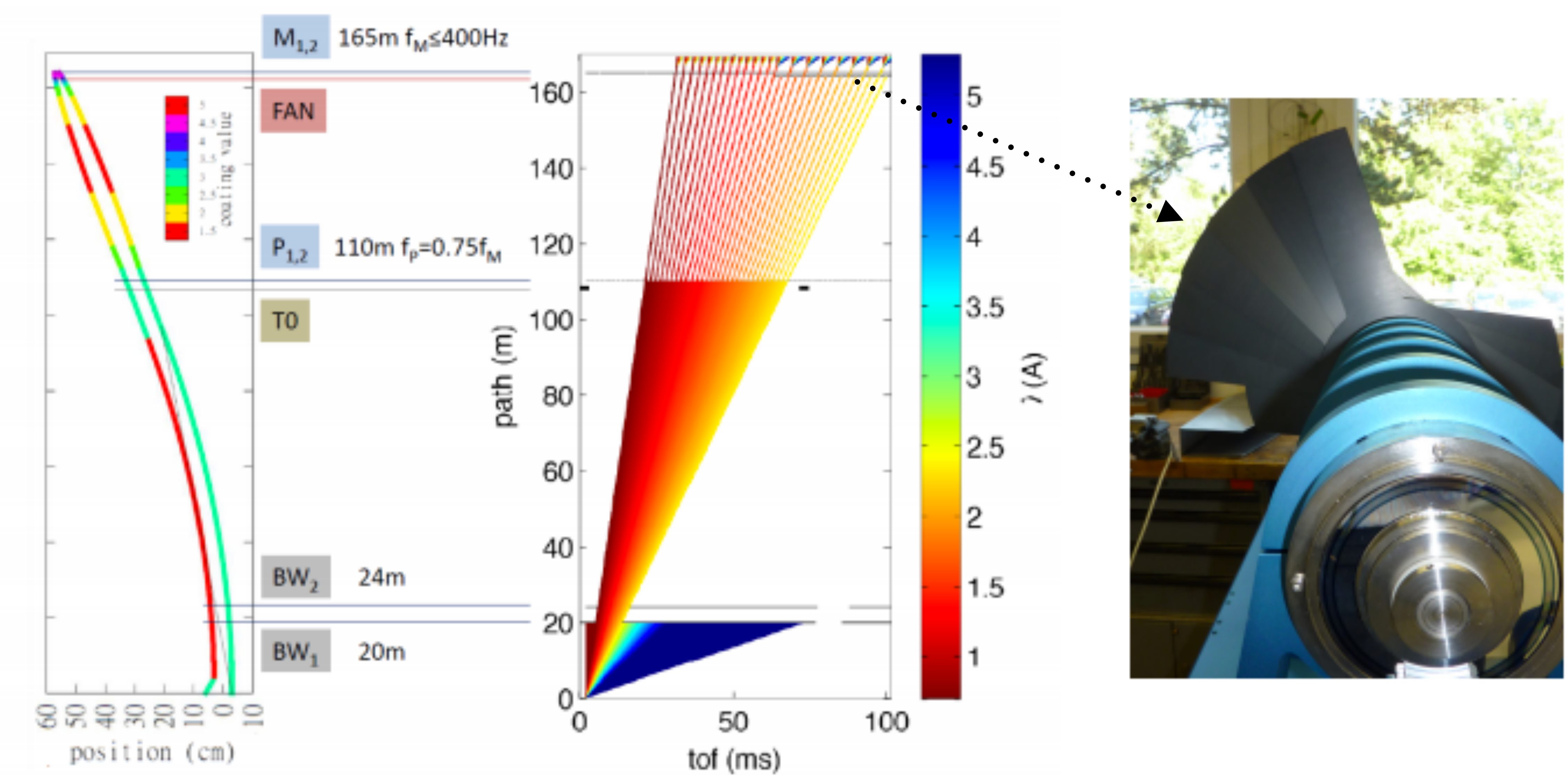
- Reduction workflows & interfaces
- Visualisation
- Detector visualisation
  - Calibration
- Integration of experiment control
  - experiment configurations and integration of hardware and DAQ

Mantid

- Mantid was a TS2 Construction project started in 2007.
- The objective was to remove single point software failures.
- Create a sustainable reduction framework.
- Handles event mode data
- Used by many existing facilities
- Works in a ‘live’ manner with ADARA type acquisition
- Currently limited to a regular geometries and stationary instruments.

Experiment control

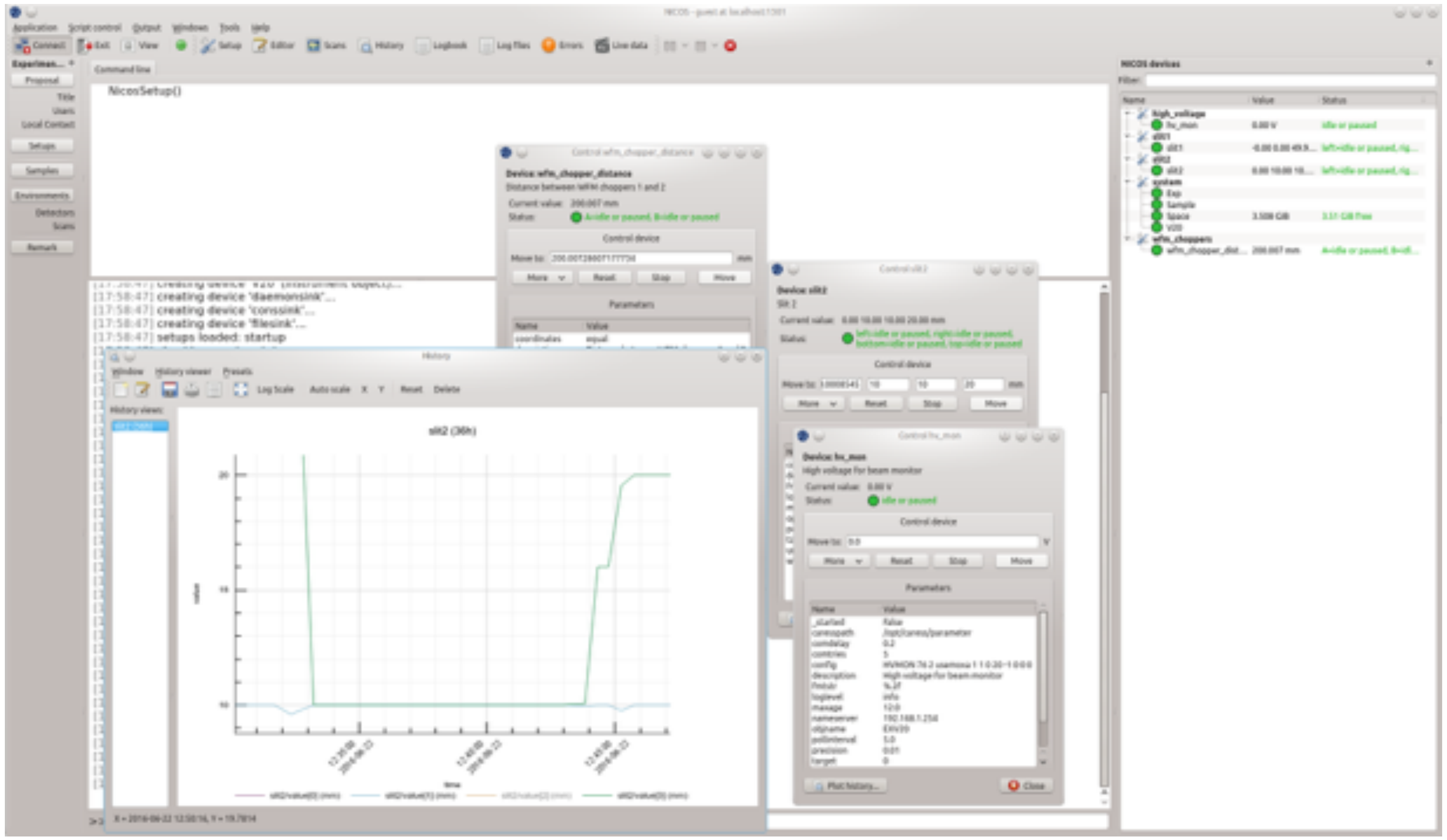
- Experiment control at ESS will be a beyond the current state of the art.
  - Instrument science cases are based on complex instrumentation
  - Complex modes of data acquisition WFM,RMM
- This complexity has to be useable and maintainable
- There is no off the shelf solution that fits all the ESS edge cases



Scientific interface

- The UI has to simplify the architecture

- Connect all the dots
  - Device control
  - DAQ control
  - Error conditions and alarms
  - Reduction / visualisation
  - Data curation cataloging
  - User office information
  - Logging and history



- NicosII is developed by TUM as a high level controls abstraction layer
- Lightweight Python framework
- Qt based GUI

Budget, scope and expectation

- The community expect excellence
- The data have to be correct
- Use of open source software is not cost neutral

Mantid development cost & schedule

- 3 releases per year
- Estimates taken from development team at ISIS and SNS
  - develop and test new workflow using existing framework including UI
    - 3-6pm
  - Same with new framework features required
    - 6-12pm
  - Core framework changes
    - 12+pm

Controls development cost and schedule

- Control roll out
  - Core development ISIS 3 years 13py effort. ~1.2M euro
  - Development replicates existing workflow.
  - Developers have combined 30+ years experience at ISIS

Comparisons

- ISIS construction projects
  - IBEX 19py development from scratch
  - Mantid ~18-20py development from scratch
  - These are numbers for core frameworks
    - No meaningful instrument / technique specific work.

- ISIS operation
  - ~18FTE developing Mantid
  - 6FTE developing IBEX for 3 instruments

13.4.3: Resource and Task Estimation

Bottom up estimate 47PY effort

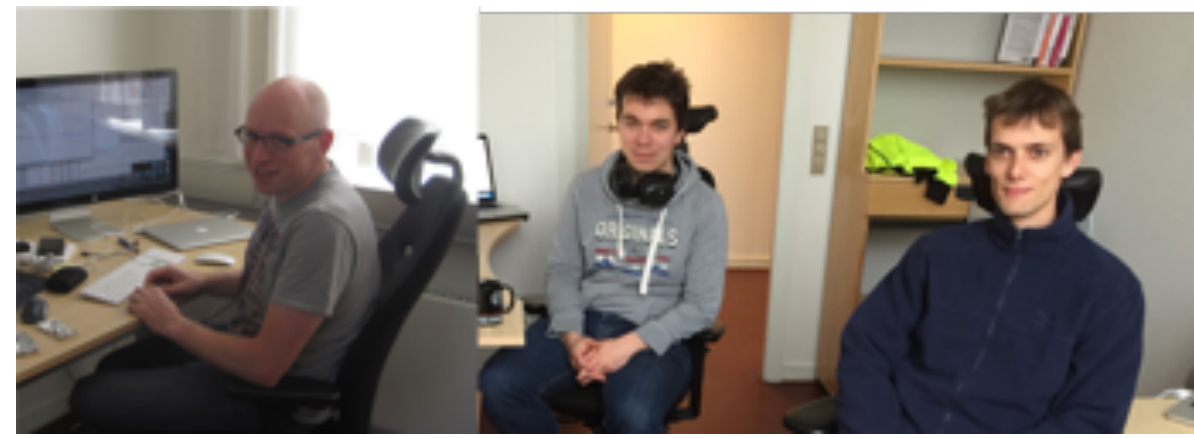
40PY available for ESS construction phase

Experiment Control	py	Cost (ESS rates)
Core FW	10	1080
LOKI	0.7	72
SKADI	0.7	72
HIEMDAL	0.7	72
DREAM	0.7	72
MAGIC	0.7	72
ODIN	0.7	72
BEER	0.7	72
CSPEC	0.7	72
TREX	0.7	72
MIRACLES	0.7	72
VESPA	0.7	72
BIFROST	0.7	72
ESTIA	0.7	72
FRIEA	0.7	72
Training	0.7	72
Documentation	0.7	108
Totals	22	2376

Data reduction & visualisation	py	Cost (ESS rate)
Core FW	8	864
Sans	1	108
Diffraction Crystal	1	108
diffraction Powder	1	108
Engineering	1	108
Imaging	1	108
Reflectometry	1	108
DG spec	1	108
indirect spec	1	108
SANS vis	1	90
Diff Vis	1	90
Imagaing Vis	1	108
DG Vis	1	108
Indirect Vis	1	90
Reflectometry vis	1	90
VATES toolkit	1	90
Training	1	108
Documentation	1	108
Totals	25	2700

13.4.3: Instrument Data Group Budget & In-Kind

	Construction Budget (M€)
Staff	1.6
Travel & Training	0.3
Experiment control inkind	1.5
Reduction inkind	2.0
Instrument data group total	5.5



ESS/DMSC core team

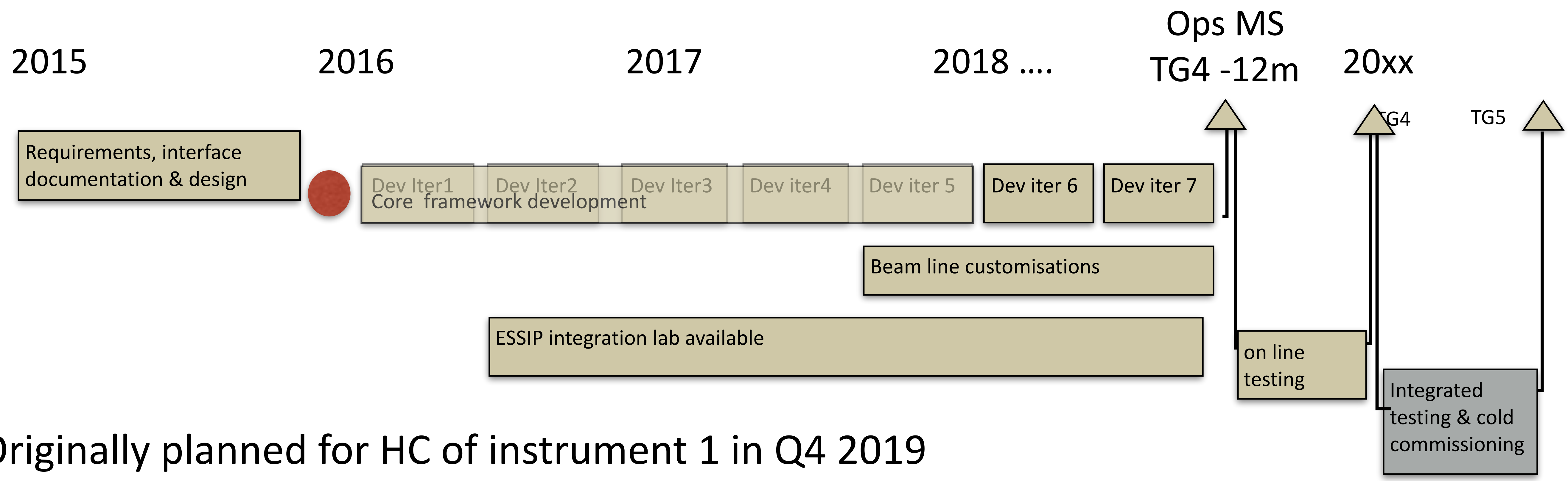
STFC ISIS In-Kind team

Core team employed at ESS

STFC in-kind agreement Started 1st Jan 2016

PSI 1.5M euro agreement for experiment control development agreed (PSI & ESS)

13.4.3: Instrument Data Group High Level Schedule



Originally planned for HC of instrument 1 in Q4 2019

~24m of core development of reduction and controls framework followed by instrument / science area tasks

Instrument / science area tasks should mirror instrument schedule -12m

The lack of a defined instrument construction schedule will soon become a planning issue

Questions

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