EUROPEAN SPALLATION SOURCE

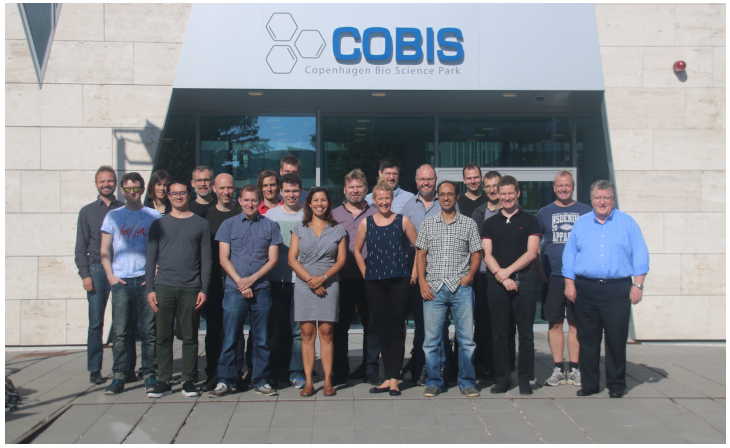
diffraction software workshop

Data Management and Software Centre

Provide world leading scientific software and scientific computing support for neutron scattering at ESS

Scientific Software development.

- ➢ The ESS experiment control system
- ➢ Data acquisition software.
- ➢ Data correction software.
- ➢ Data visualization software.
- ➢ Software to model and analyze experimental data



DMSC offices located at COBIS. Copenhagen University north campus

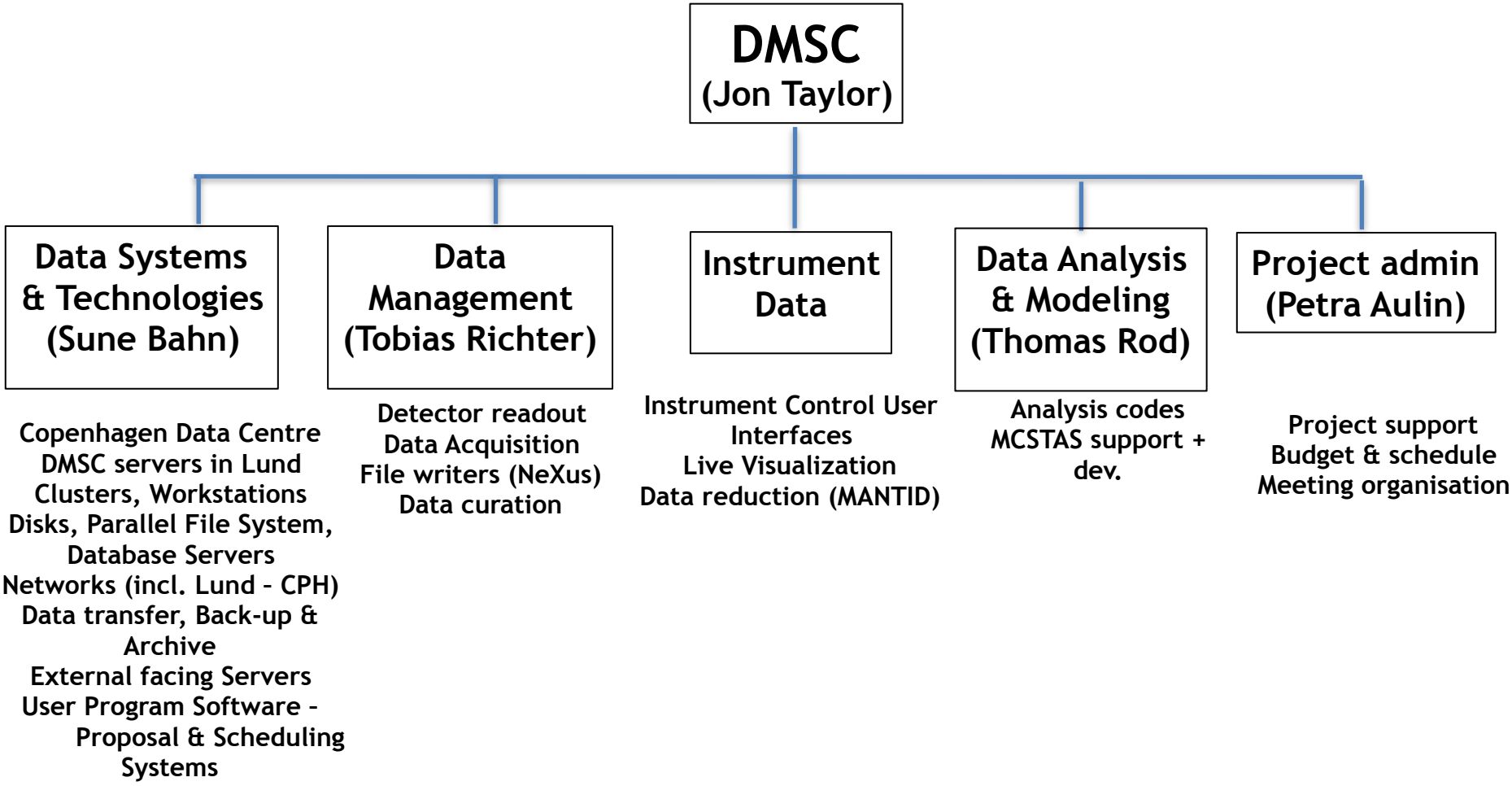
Data centre operations.

- ➢ Store & catalogue ESS neutron datasets.
- ➢ Provide ESS users remote access to their data
- ➢ Compute provisioning for live data correction, visualization and analysis software during and after experiments.

User programme support (operations phase)

- ➢ Provide support & assistance to ESS users for data treatment and data analysis.

DMSC Organization



DMSC construction budget

- 20M euro + SINE2020 (42 pm) + Brightness (23 py)

- Software development
- Detector read out, Data Acquisition, Data management

- Experiment control core framework
- Live data reduction & visualisation framework

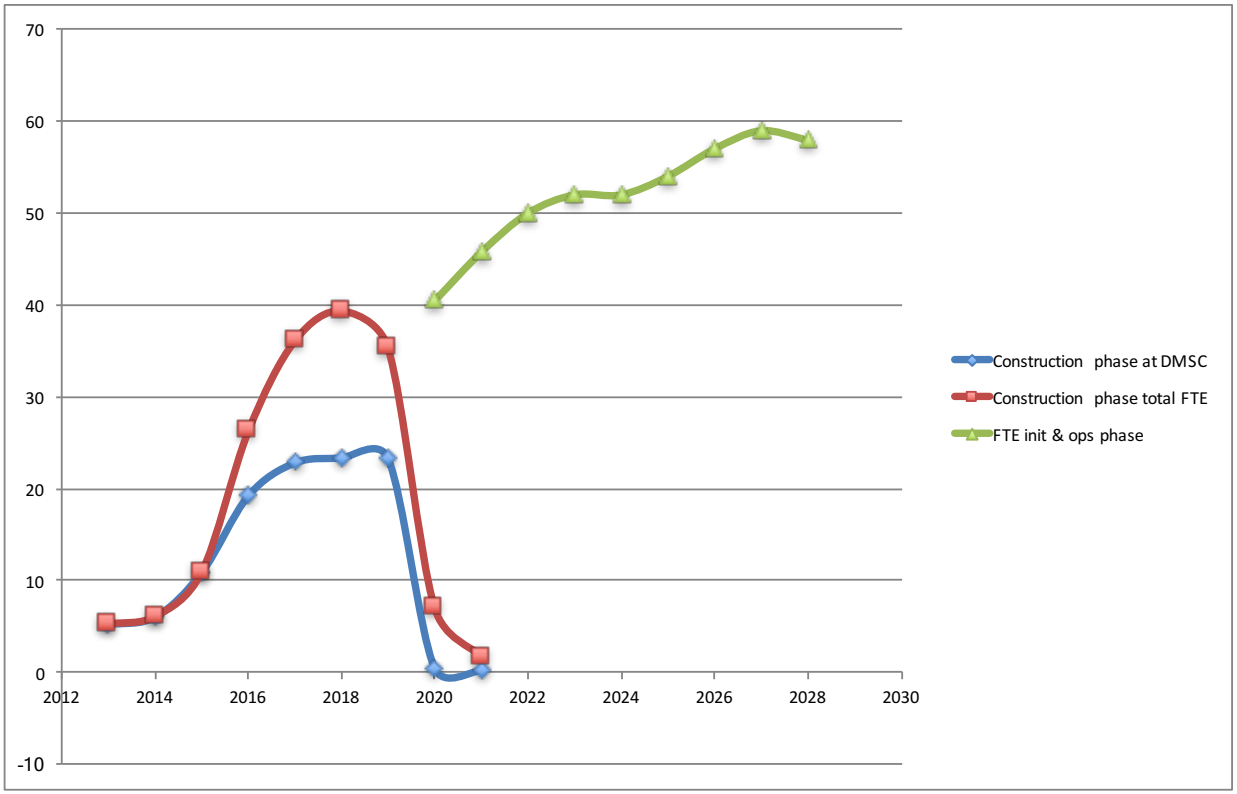
- Data analysis core codes framework development

- Operation of ESS cluster
- Initial storage solution & compute hardware

- (User office software development)

DMSC Current staff profile & budget

- Budget 20M euro
- Mixture of core staff in-kind and external funding
- Brightness 25py and in-kind 43py



Instrument software meetings

Charge:
Outline & agree the core requirements* for instrument control
Outline & agree the core requirements for data reduction
Outline & agree the core requirements for data analysis
Provide a realistic time line into full operations of diffraction instruments for DMSC.
*core requirements are provided within the DMSC budget for construction, more with operations funding beginning in 2019.

- DSMC STAP and Instrument teams

- Reflectometry 21st March
- Diffraction April 7th
- Imaging 26th-27th April
- SANS 1st - 2nd June
- Spectroscopy 15th May

Instrument software delivery projects

- Tie specific DMSC deliverables to instrument schedule

- 1 instrument 1 project
  - Capture all DMSC related deliverables
  - DAQ, Control, Reduction, Analysis, data management
  - Generate milestones for delivery

- Define essential ‘must have’ requirements
- Define completion
- 6m update meetings
- No funding for unwanted development

What is already decided

- Overall DAQ / controls architecture
  - Controls & DAQ technologies
  - Data flow
- Centralised compute & data storage
  - Hardware in Lund and Copenhagen
- Data reduction f/w Mantid
- Experiment control f/w Nicos2
- Construction phase scope

Key milestones for project delivery

Detector readout & DAQ chain for testing (with source)
Detector readout & DAQ chain for testing / commissioning with neutrons
Detector readout & DAQ for user programme

Controls & functionality ready for cold commissioning
Controls & Controls functionality ready for hot commissioning
Experiment Control functionality ready for user programme

Data reduction / visualisation ready for commissioning (source) or hot commissioning
Data reduction functionality ready for early science
Data reduction and visualisation ready for user programme

Data reduction functionality ready for user programme
Data analysis functionality ready for early science
Data analysis functionality ready for user programme

Compute requirements for cold —> hot commissioning
Storage requirements available for commissioning (Hot & Cold)
Storage requirements available for user programme.
UX & Remote access functionality ready for user programme

Construction scope reduction & Control.

- Construction phase ends Dec 31st 2019
- Core data reduction functionality
- Core experiment control functionality

- Operations scope
  - Instrument specific requirements developed from 2020.

Data rate

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- ESS average rate is ~8GB /min

- Data reduction will be run on a cluster
  - 75% of construction phase mantid development is performance improvements.

- What does this data rate mean for diffraction ?
- Automated reduction
- Workflow

User experience

- What should we aim for at the various stages

- Commissioning
- Early use
- User programme

- User interaction with DMSC systems
- Automatic reduction
- Visualisation
- Automated analysis

- Remote access

Data acquisition & control

- DAQ synced to accelerator 14Hz pulse
- Event mode data collection
- All neutron & meta data timestamped from ESS central timing system
  - Timing system is delay compensated
- Neutron event data is aggregated with metadata on a frame by frame basis
- 71ms Latency
- Frames of data on a pub / sub network
- Vetos and meta data filtering are performed in software

- What are the expected operational modes
  - Commissioning & user programme

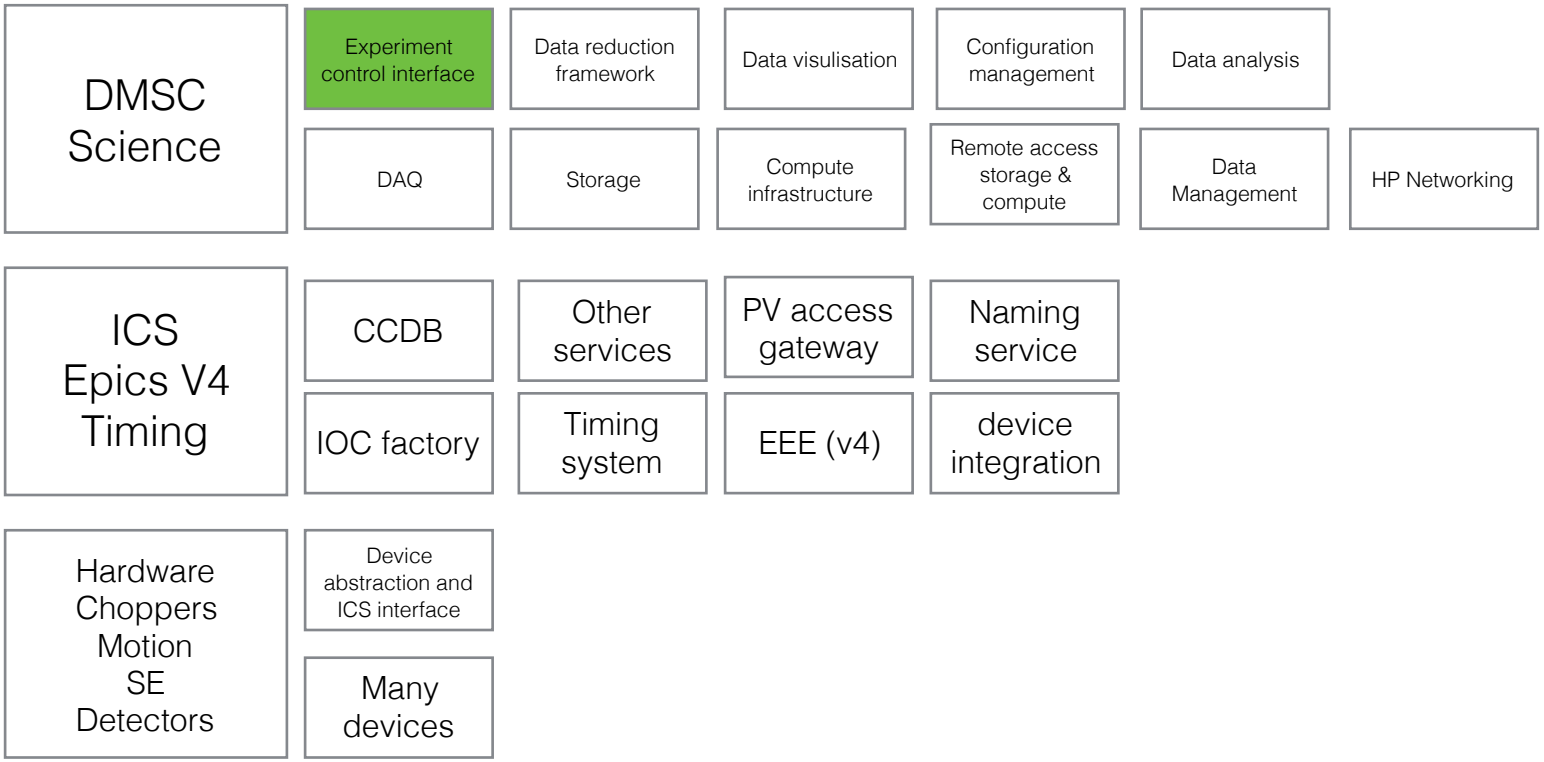
Data reduction and visualisation

- Mantid has various diffraction workflows for SNS & ISIS
- What's missing ?
- How should we deal with polarisation states & event data
- Visualisation
  - What is required
- What is the performance requirement
- How much data is expected per day / per experiment
- What planning tools are required to make this efficient.

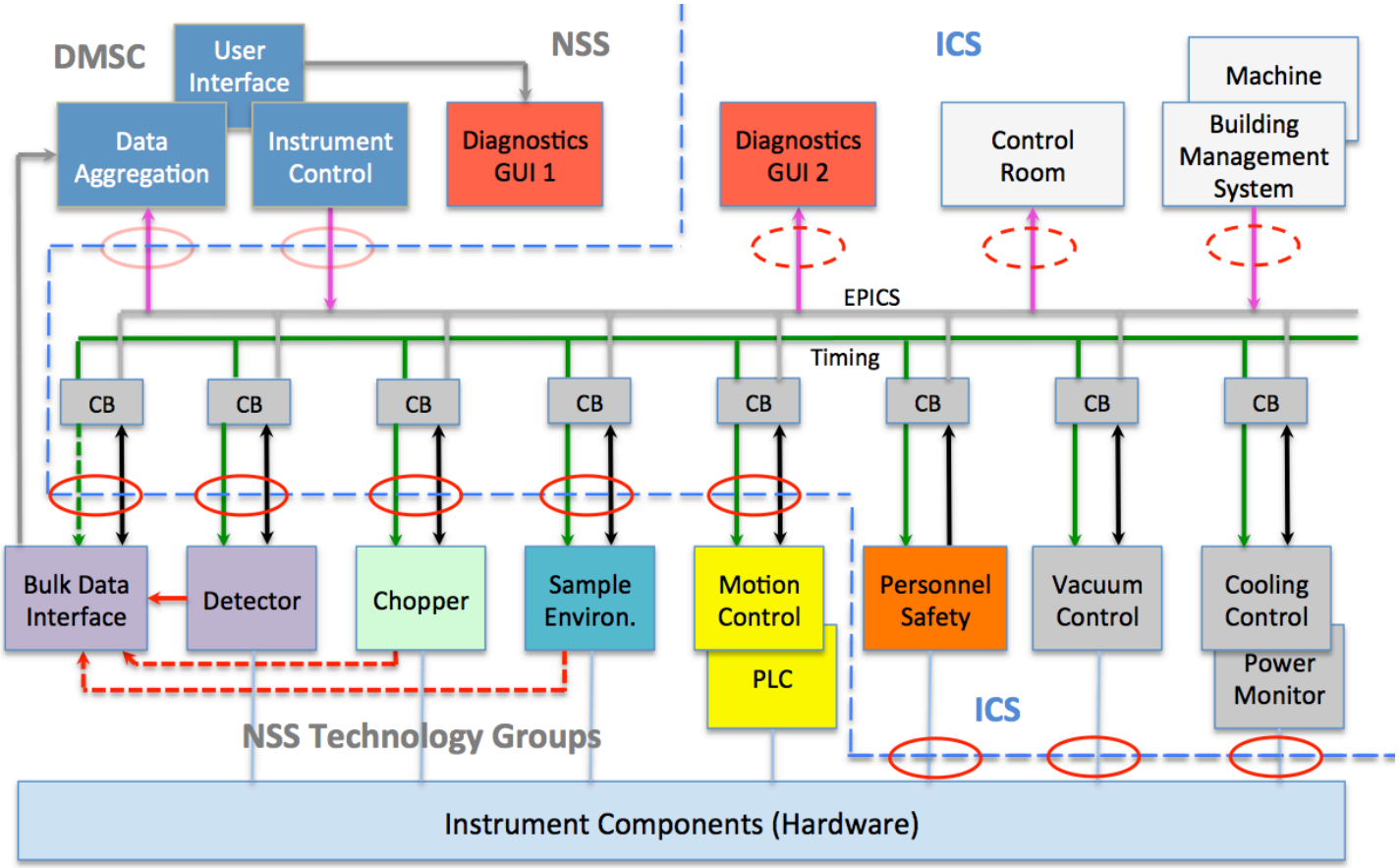
additional slides

Experiment control

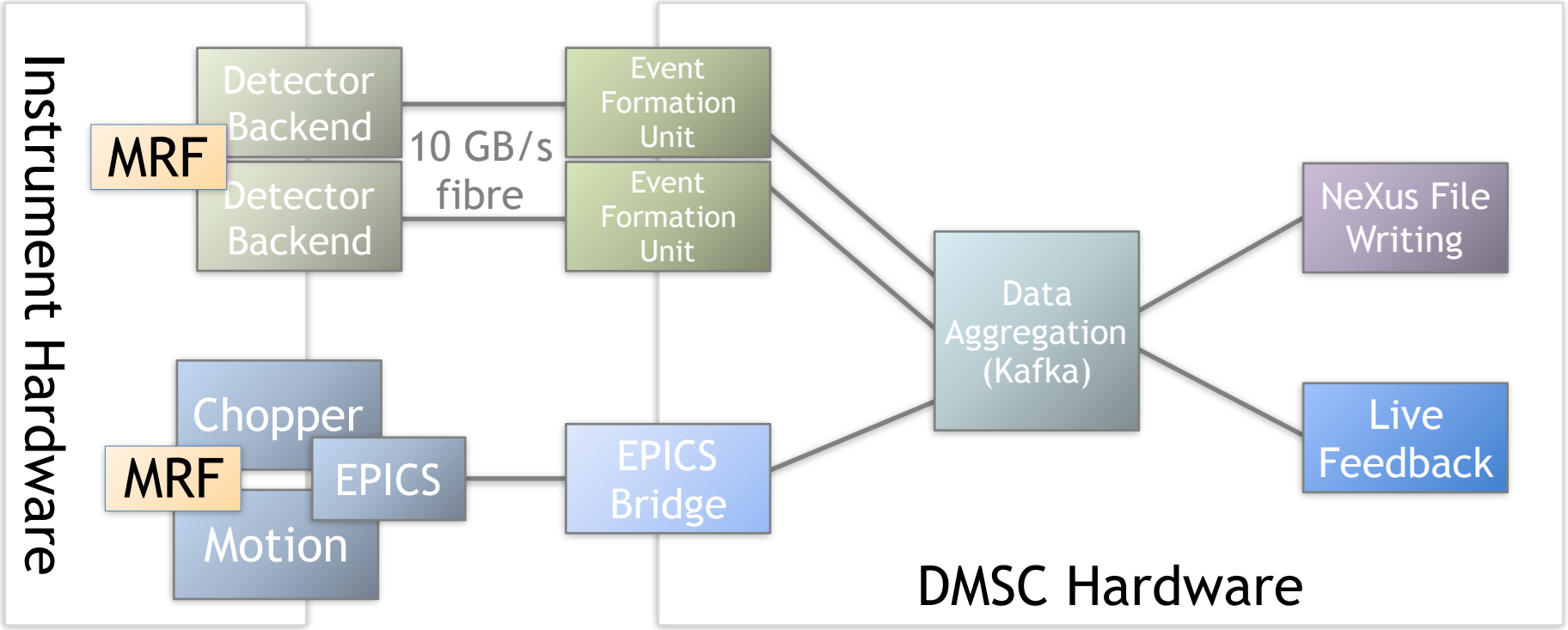
- Device abstraction layer is EPICS
- Experiment control layer will be python based NICOSII
- utilising a number of tools to deploy epics control onto instruments
- Experiment control at ESS will be a beyond the current state of the art.
    - Instrument science cases are based on complex instrumentation
    - Complex modes of data acquisition WFM,RMM
- This complexity has to be useable.
- There is no off the shelf solution that fits all the ESS edge cases



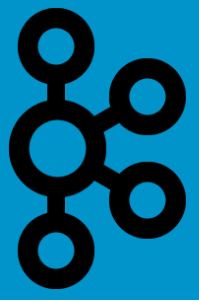
Controls layout



Readout Architecture



BrightnESS is funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 676548



APACHE kafka™

A distributed streaming platform

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PUBLISH & SUBSCRIBE

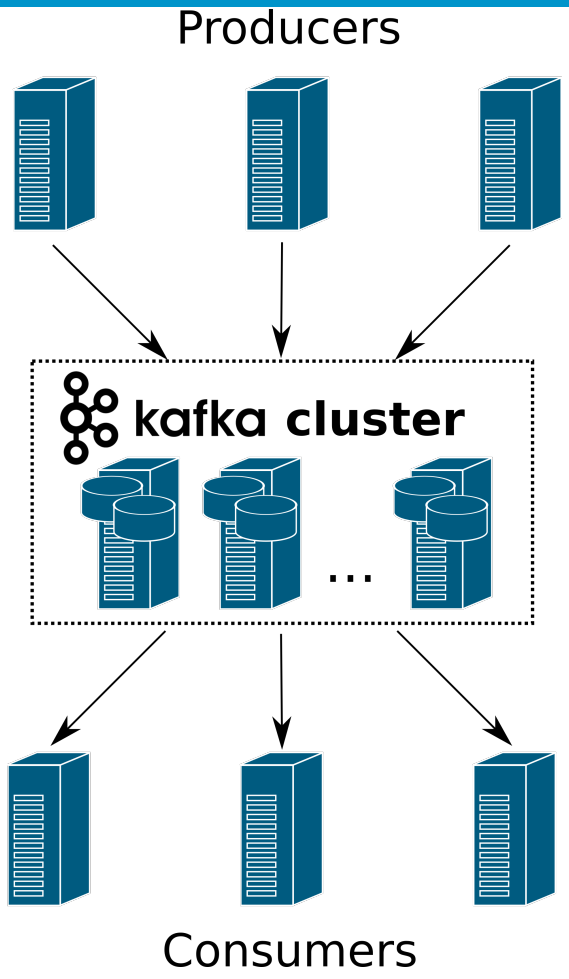
to streams of data like a messaging system

STORE

streams of data safely in a distributed replicated cluster

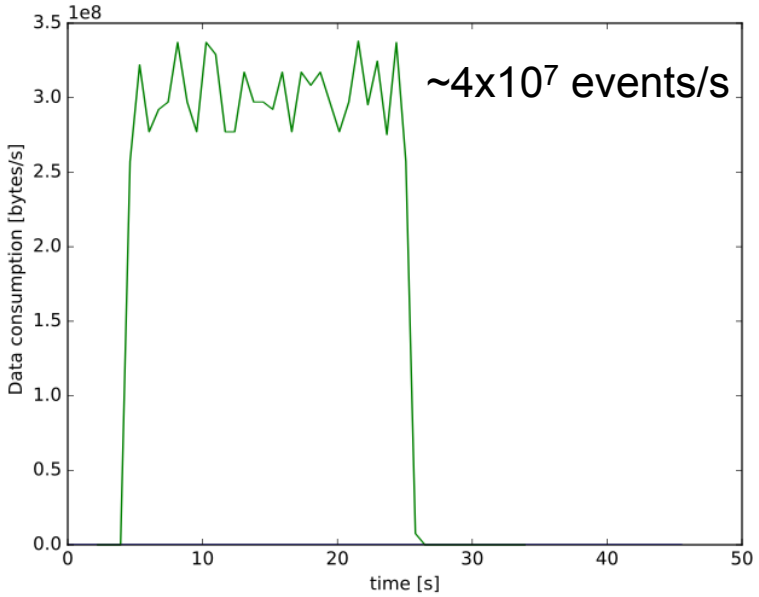
Kafka for DAQ

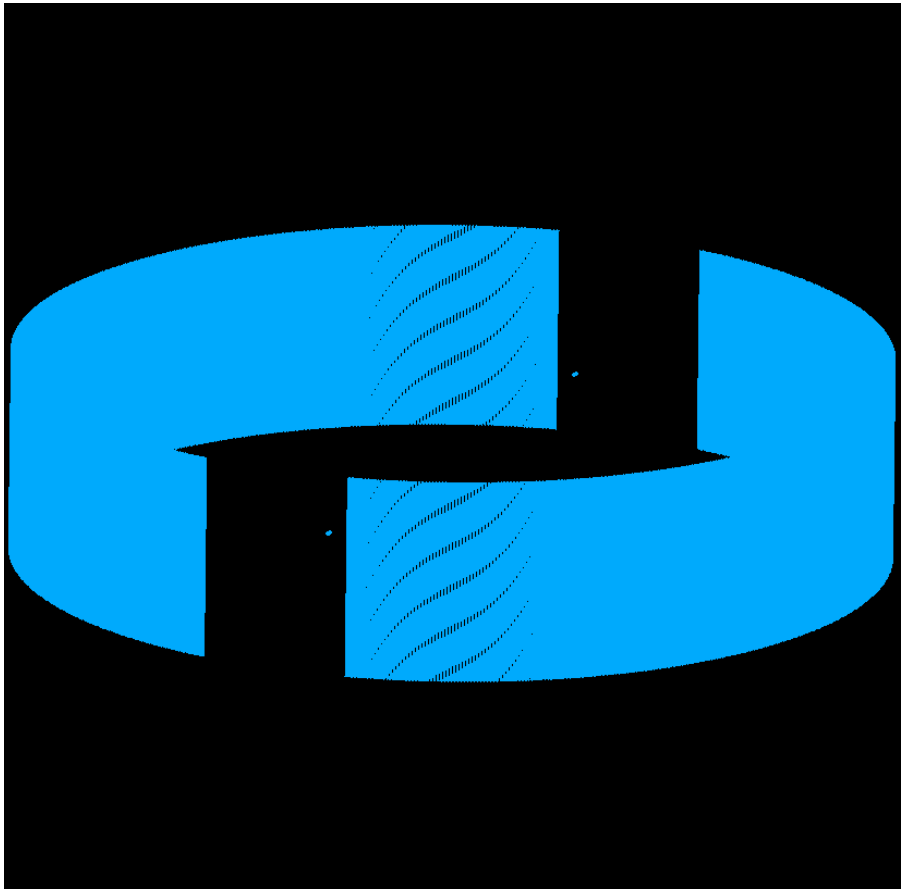
- Detectors
- Aggregator
- File writer
- Live / auto reduction



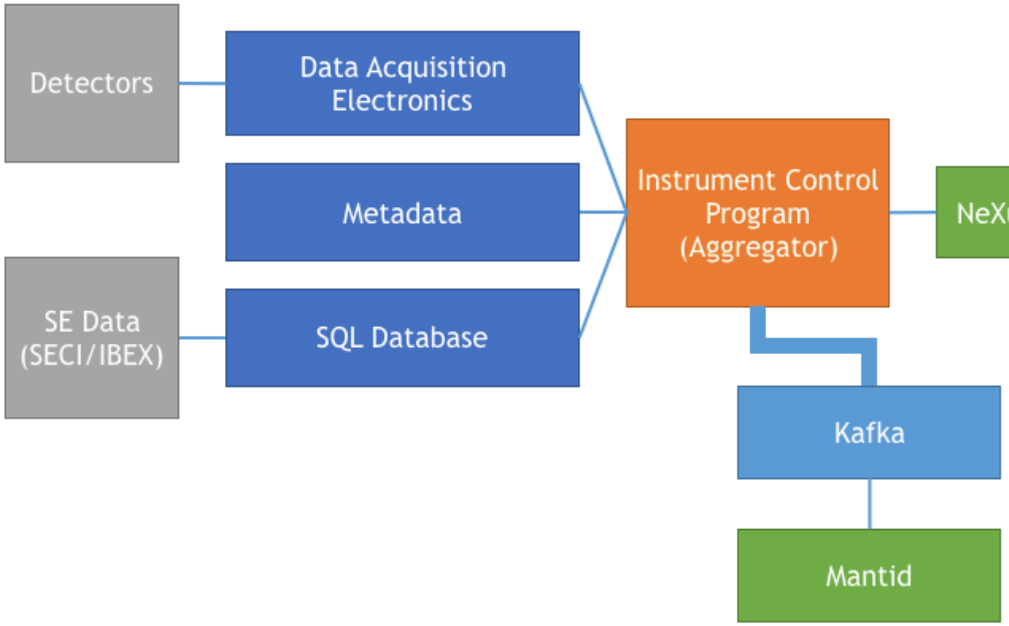
Proof of concept: historical data

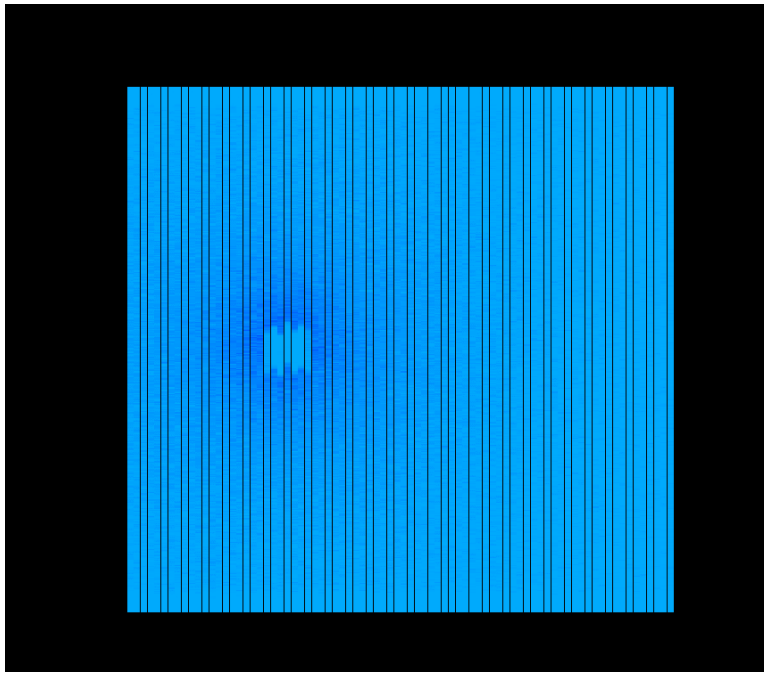
- Streaming a NeXus file through Kafka to Mantid
- Scaleable performance





Test in live environment





The Mantid Project

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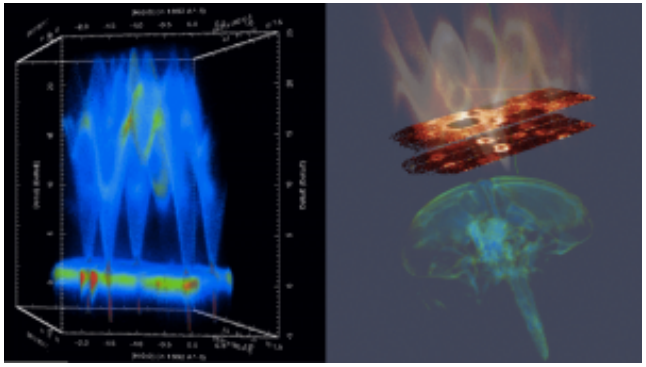
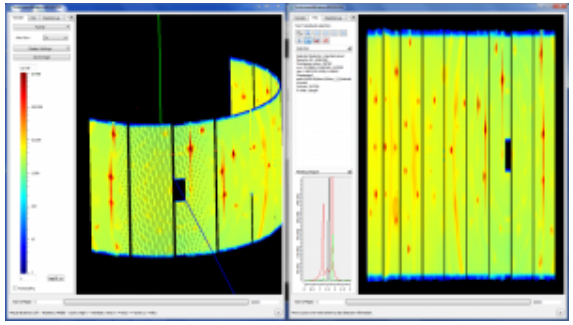
MANTID



- Neutron specific data treatment framework
- Standardised beyond data format
- Event data capable
- Live view
- Complete instrument geometry
- nD data visualisation
- Data and software curation
- App based UI
- Python interace
- Jupyter notebook
- MPL graphing

ParaView



ISIS

OAK RIDGE National Laboratory

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NEUTRONS FOR SCIENCE

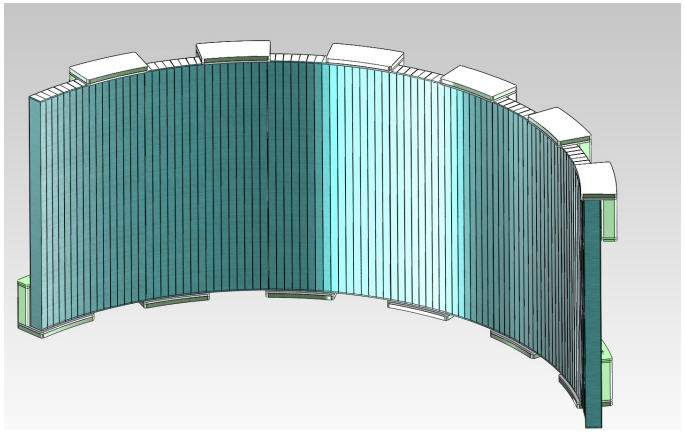
Tessella Technology & Consulting

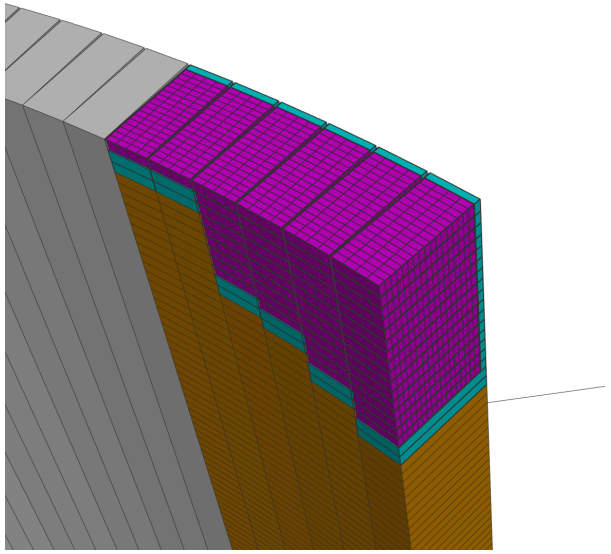
ansto

PAUL SCHERRER INSTITUT PSI

Mantid Performance requirements

- Requirements -
  - live data reduction for an event rate of > 10^7
  - Filter good events from bad events
  - Capability for handling of complex geometries

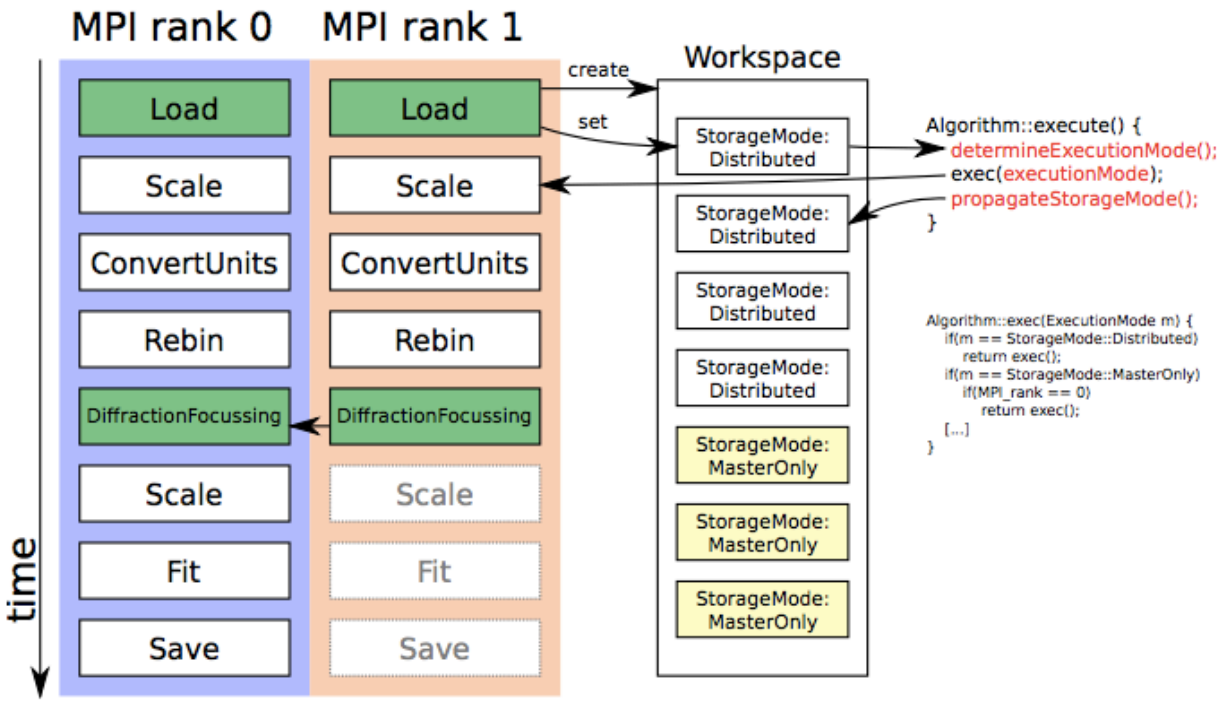




Mantid development objectives

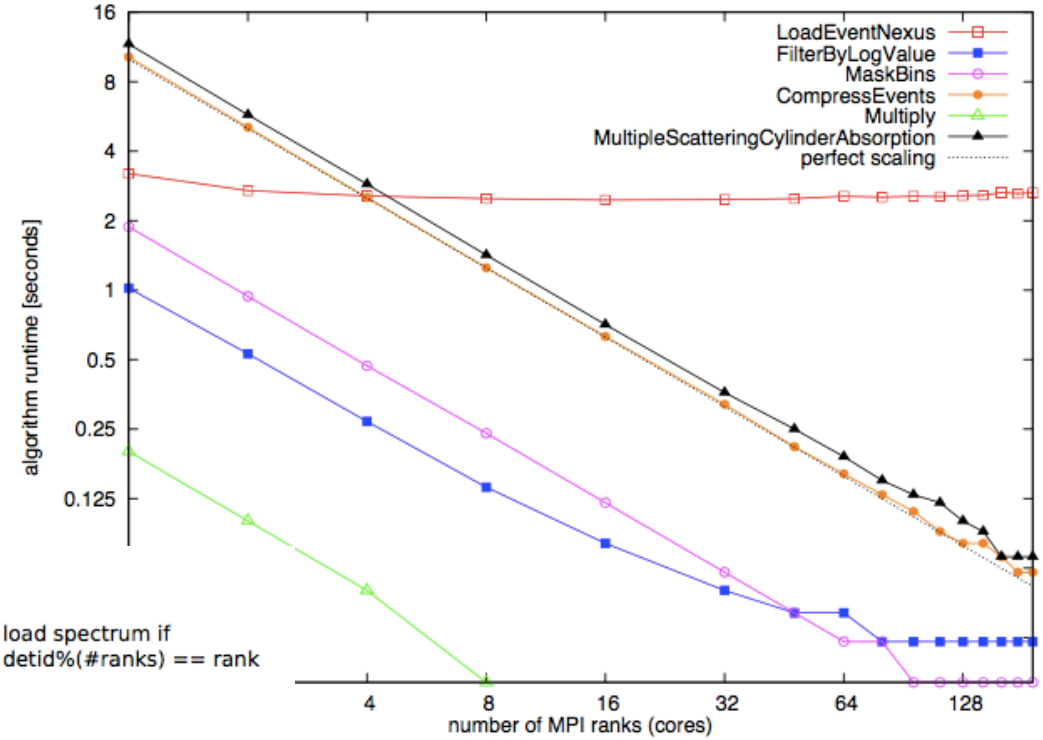
- Mantid has
  - Geometry
  - Data types
  - algorithms

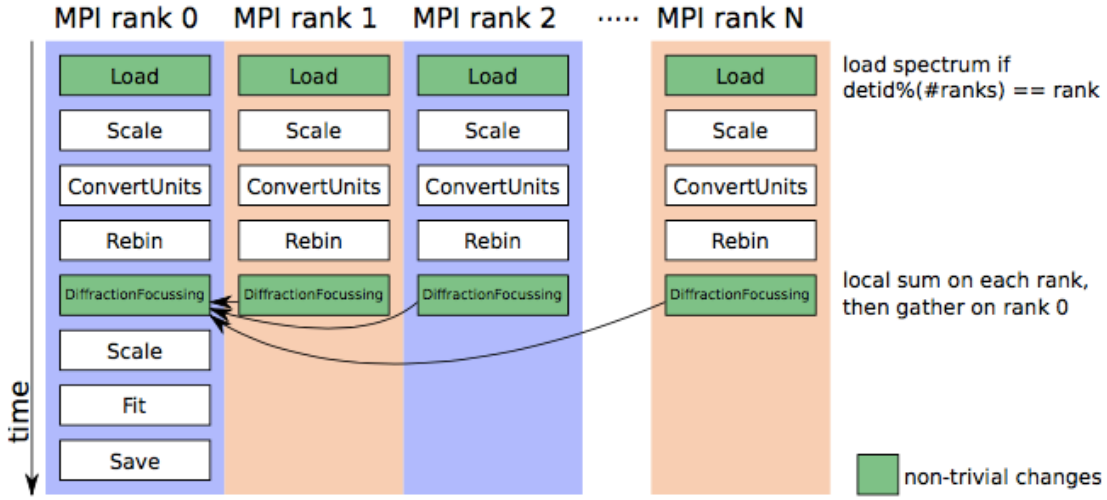
- Create a common MPI implementation
- Introduce type safety



Initial MPI tests

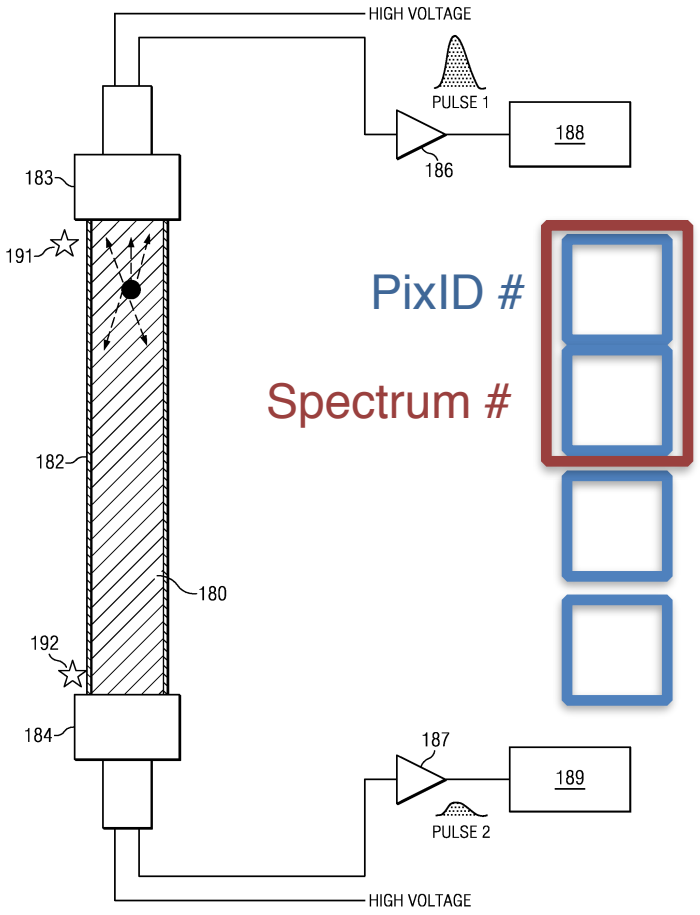
- MPI more effective than threads.
- A number of ways to achieve load balance
- We balance on spectra





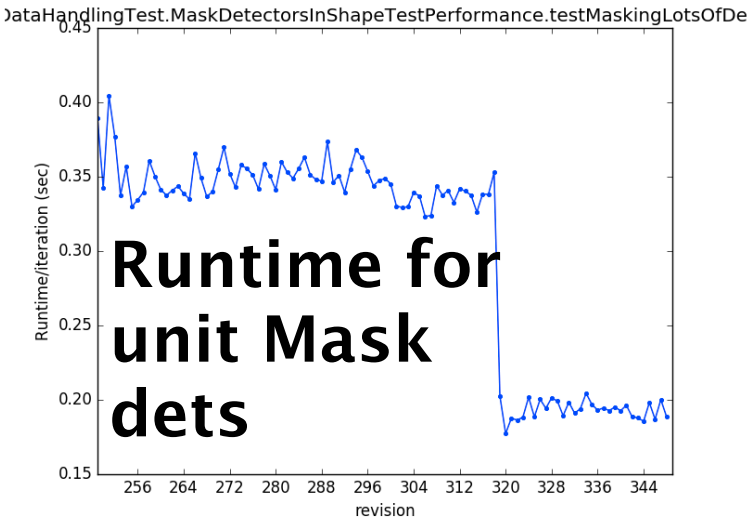
Instrument 2.0

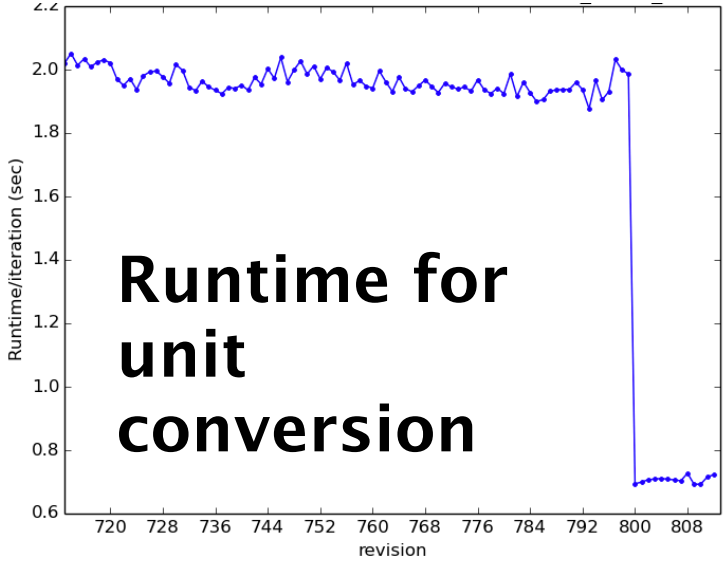
- Instrument stores geometry and meta data.
- r,t,p spectrum ID map, isMasked…
- Complex detector geometries
- Described within the framework
- Current Instrument implementation is limiting
  - Parameter map is large /complex
  - Organically developed



so far so good…

- Highlights the cost of refactoring
- Significant improvements across Mantid
- ILL can load interlaced scans from D2B into Matrix
- Direct geometry workflow x2 faster





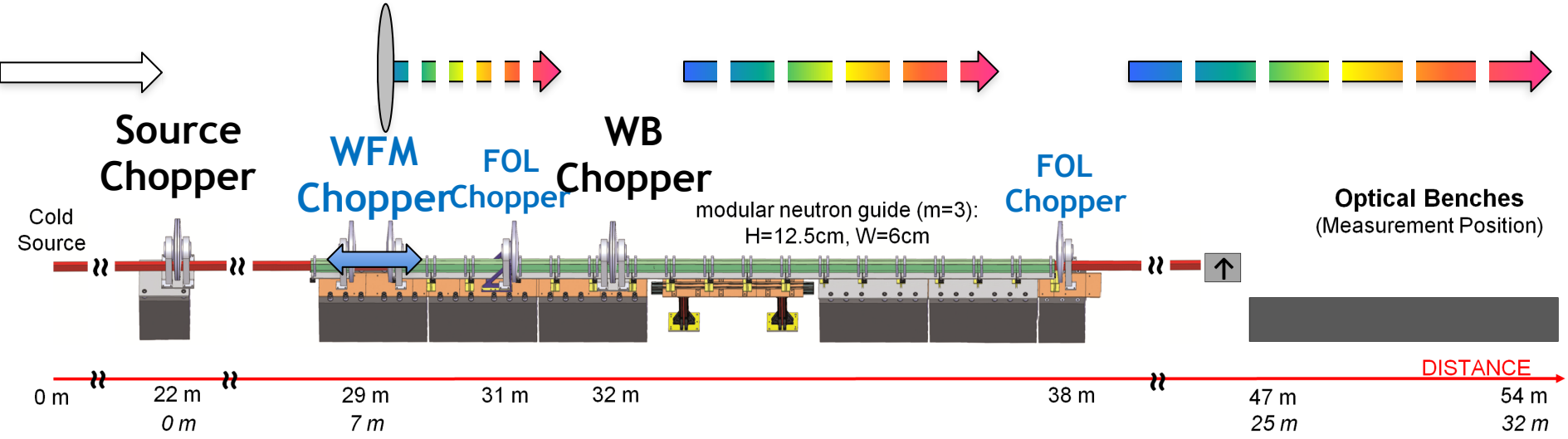
Experiment control progress

- Data chain is well described
- All scope is covered by DMSC / ICS / NT / SAD

- Experiment control project
  - DMSC + ISIS in-kind + PSI in-kind
  - ICS + SAD
  - Steering committee for all stakeholders
  - Instruments represented by Andrew Jackson
- PDD ESS0102794

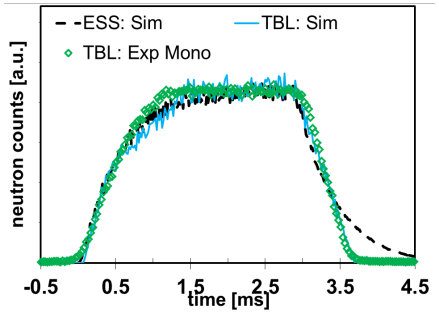
- Base framework will be NICOS2
- Deployed on V20 TBL

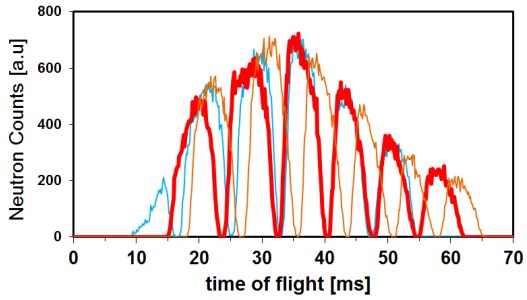
V20 Test beam line



- ☑ Experiment control integration
- ☑ WFT data reduction tests
- ☑ User experiments with Nicos

- ○ Integration with ICS EEE systems





Experiment control