



nmi3

Data Analysis Standards (WP6)

ILL (lead), STFC/ISIS, TUM and JCNS (FRM2), PSI, HZB, CEA LLB,
HZG/Hamburg, ESS Lund/Copenhagen

<<http://nmi3.eu/about-nmi3/networking/data-analysis-standards.html>>

Workpackage current status

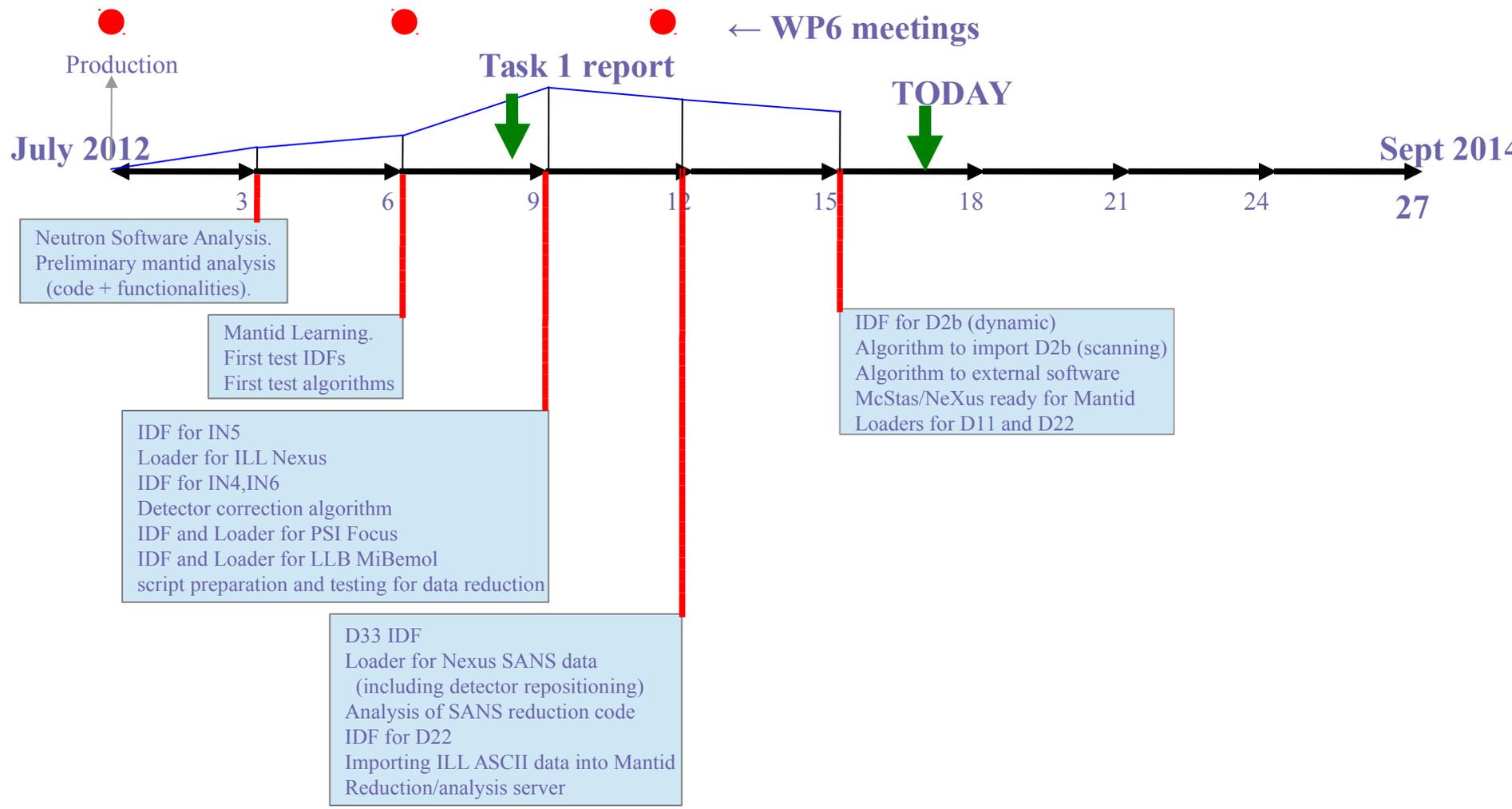
Task 3 items 'Develop prototype software in chosen solution for representative applications'

- Contributions to Mantid: instruments, McStas

Task 2 'Review existing solutions for a common data analysis infrastructure'

- Live data analysis
- Live DVD and package repository

WP6 - current status



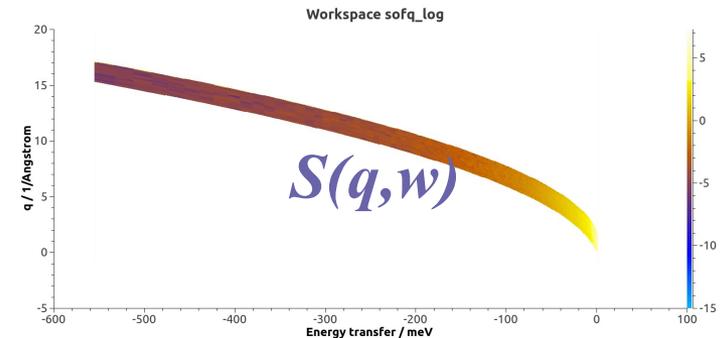
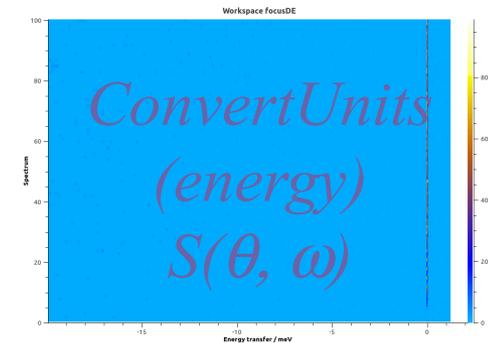
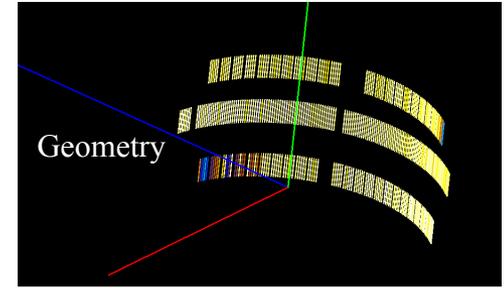
Mantid: PSI Focus (ToF)

Done:

- Instrument geometry (IDF) fixed
- Importer OK
- Corrections for the detector parallax and efficiency OK
- Possibility to use any ToF algorithm, e.g. ConvertUnits, SofQW
- ILL IN4 and IN6
- LLB MiBémol

Pending:

- FRM2 ToFToF
- HZB NEAT



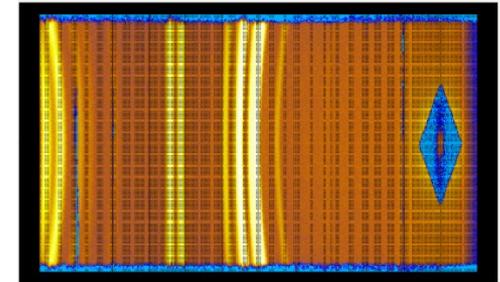
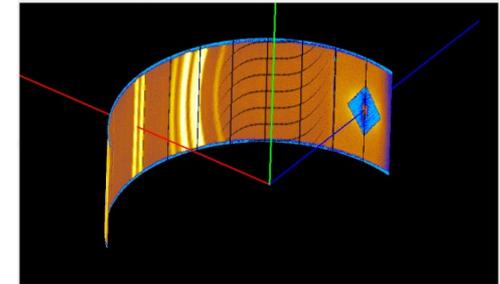
Mantid: ILL IN5 (ToF)

Done:

- Instrument geometry (IDF) fixed
- Importer OK
- Corrections for the detector parallax OK
- Possibility to use any ToF algorithm, e.g. ConvertUnits, SofQW

Pending:

- No link with VATES yet for single Xtal



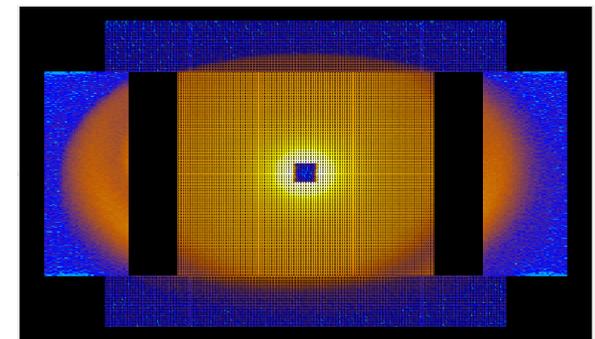
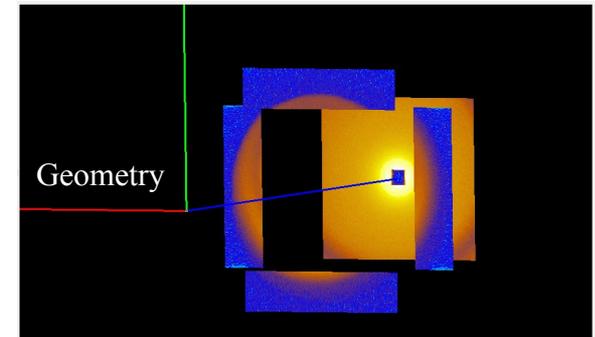
Mantid: ILL D33 (ToF SANS)

Done:

- Instrument geometry OK
- Importer OK
- Ready for ILL D11 and D22

Pending:

- Issue with two implementations for SANS algorithms / GUIs (SNS vs. ISIS)
- Trips to ISIS (Dec) and SNS (Jan) planned
- Should be OK for series of acquisitions
(not fixed but not scanning → group for e.g. stop-flow cells)



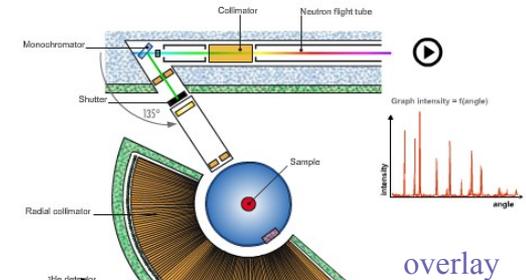
Mantid: ILL D2B (HR powder diffractometer)

Done:

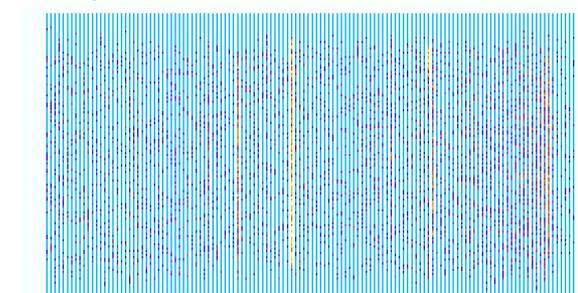
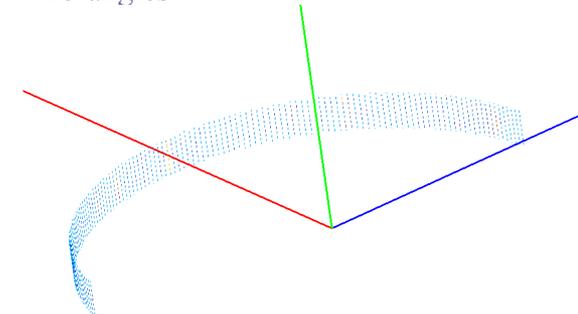
- Instrument geometry OK
- Data importer for a single scan step

Pending:

- How to merge different geometries ?
- No detector corrections yet
- Solve this case before switching to e.g. TAS (complex scanning)



Scan
25 angles





Mantid: interface to McStas (ILL and DTU/Risoe)

Done:

- McStas geometry exported to an IDF for Mantid
- Loader for McStas NeXus result files (events, histograms)



Pending:

- Still experimental, but promising

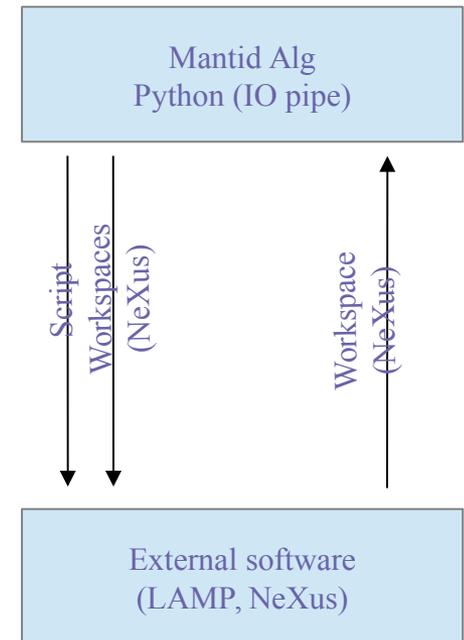
Mantid: interface to other software (LAMP,iFit)

Done:

- An algorithm can send any script to an external software, and get results through a temporary NeXus file to create a workspace transparently.
 - Tested with LAMP and iFit
 - Coded in Python, not contributed (testing)
- <<https://github.com/ricleal/AllToMantid>>

Pending:

- Only seen as a temporary hack, but may be handy !





Mantid: a few thoughts

Redundancy in algorithms makes algorithm choice sometimes tricky

- (which one ? “SANS” “SofQW”)

Python algorithms preferred (esp. for scientists)

- avoid C++ complexity, unless computational speed required

Scanning/moving instruments ‘challenges’ in Mantid framework

GIT repository – NMI3 developments continuously injected, included in Mantid project release, and packaged for distribution.

Documentation – structure and content for developers and users

Meetings for developers in Jan 2014 at SNS (user meeting attended in September 2013)

Mantid/NMI3 – attempt to rationalise **data reduction** software (share more & duplicate less)

Data analysis is more diverse – a number of key pieces of software must be identified and supported collectively

Data pipeline (acquisition/reduction/analysis) must be created from several ‘modules

→ NMI3 ‘data analysis’ meeting in 2014

Testing a prototype shared repository:

- <<http://packages.neutroncode.org>> for e.g. Debian/Linux – (currently 25 packages, neutron oriented)
- Could be generalized to Mac and Windows (**wpkg**)
- Distribute a LiveDVD built with these packages (updated July 2013)

Prototype for a distant computation server

Computation triggered from e.g. instrument control or web page

Uses a dedicated communication port to exchange requests and data

Allow to plug any computation client

<<https://github.com/ricleal/reductionServer>>

Implemented with NoMAD@ILL $\leftarrow \rightarrow$ Server $\leftarrow \rightarrow$ Mantid, iFit, LAMP,...

