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

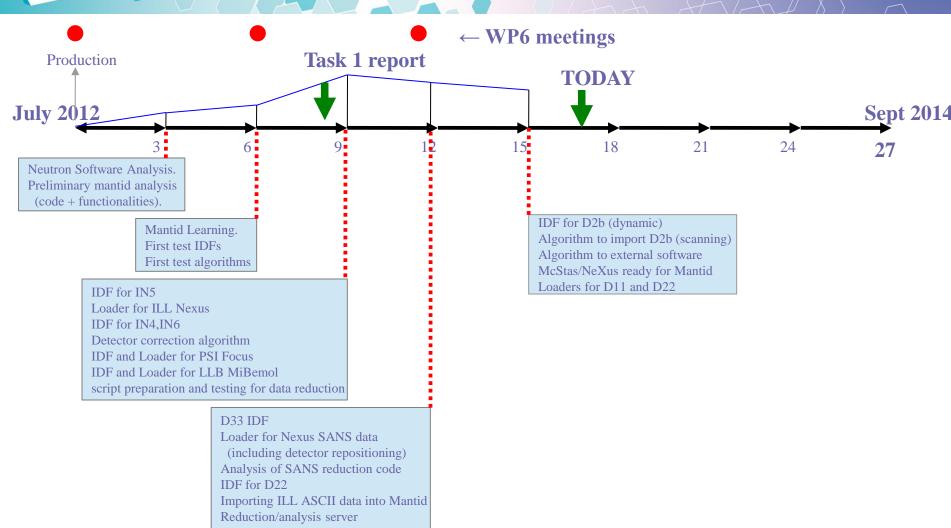## Task 3 items 'Develop prototype software in chosen solution for representative applications'

- 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
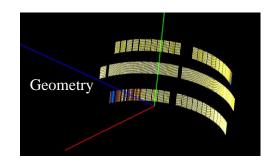

← WP6 meetings

Production

Task 1 report

TODAY

July 2012

Sept 2014

3 6 9 12 15 18 21 24 **27**

Neutron Software Analysis.
Preliminary mantid analysis
(code + functionalities).

Mantid Learning.
First test IDFs
First test algorithms

IDF for IN5
Loader for ILL Nexus
IDF for IN4,IN6
Detector correction algorithm
IDF and Loader for PSI Focus
IDF and Loader for LLB MiBemol
script preparation and testing for data reduction

D33 IDF
Loader for Nexus SANS data
  (including detector repositioning)
Analysis of SANS reduction code
IDF for D22
Importing ILL ASCII data into Mantid
Reduction/analysis server

IDF for D2b (dynamic)
Algorithm to import D2b (scanning)
Algorithm to external software
McStas/NeXus ready for Mantid
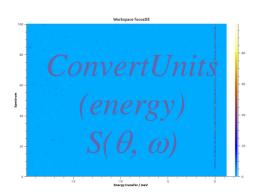Loaders for D11 and D22
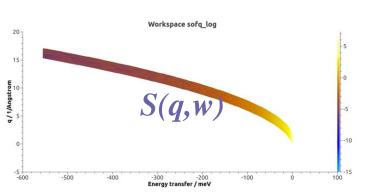
Mantid: PSI Focus (ToF)

Geometry

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

ConvertUnits (energy)
$S(\theta, \omega)$
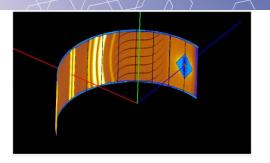
Pending:
- FRM2 TofTof
- HZB NEAT

$S(q,w)$

Mantid: ILL IN5 (ToF)

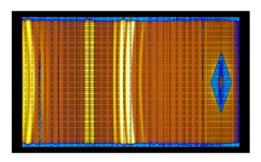**Done:**
- Instrument geometry (IDF) fixed
- Importer OK
- Corrections for the detector parallax OK
- Possibility to use any ToF algorithm, e.g. ConvertUnits, SofQW
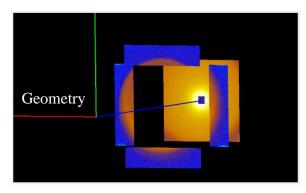
Pending:
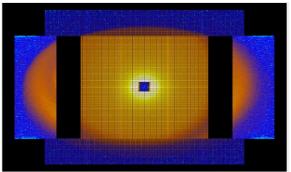- No link with VATES yet for single Xtal

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
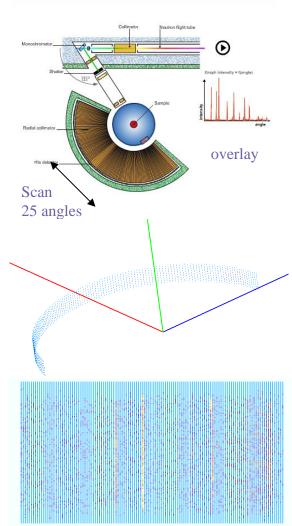- Should be OK for series of acquisitions (not fixed but not scanning → group for e.g. stop-flow cells)

Geometry

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)

overlay

Scan
25 angles

Task 3: Prototype Software

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)
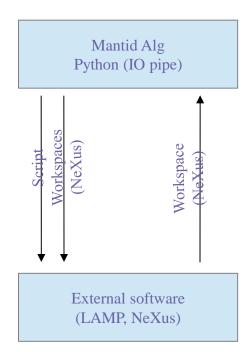
Pending:
- Still experimental, but promissing

Task 3: Prototype Software

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 Alg |
| Python (IO pipe) |

Script
Workspaces (NeXus)

Workspace (NeXus)

| External software |
| (LAMP, NeXus) |

iFit

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)

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 ← → Server ← → Mantid, iFit, LAMP,...

Instrument Control PC
(e.g. NoMad)

Live Data Analysis Server

Data treatment
(i.e. LAMP, Mantid, iFit, etc)

HTTP POST Data file

HTTP POST Query

Call data processing routine

Return QueryID

Send to the server the routine results

HTTP GET Results for QueryID

Return Results