

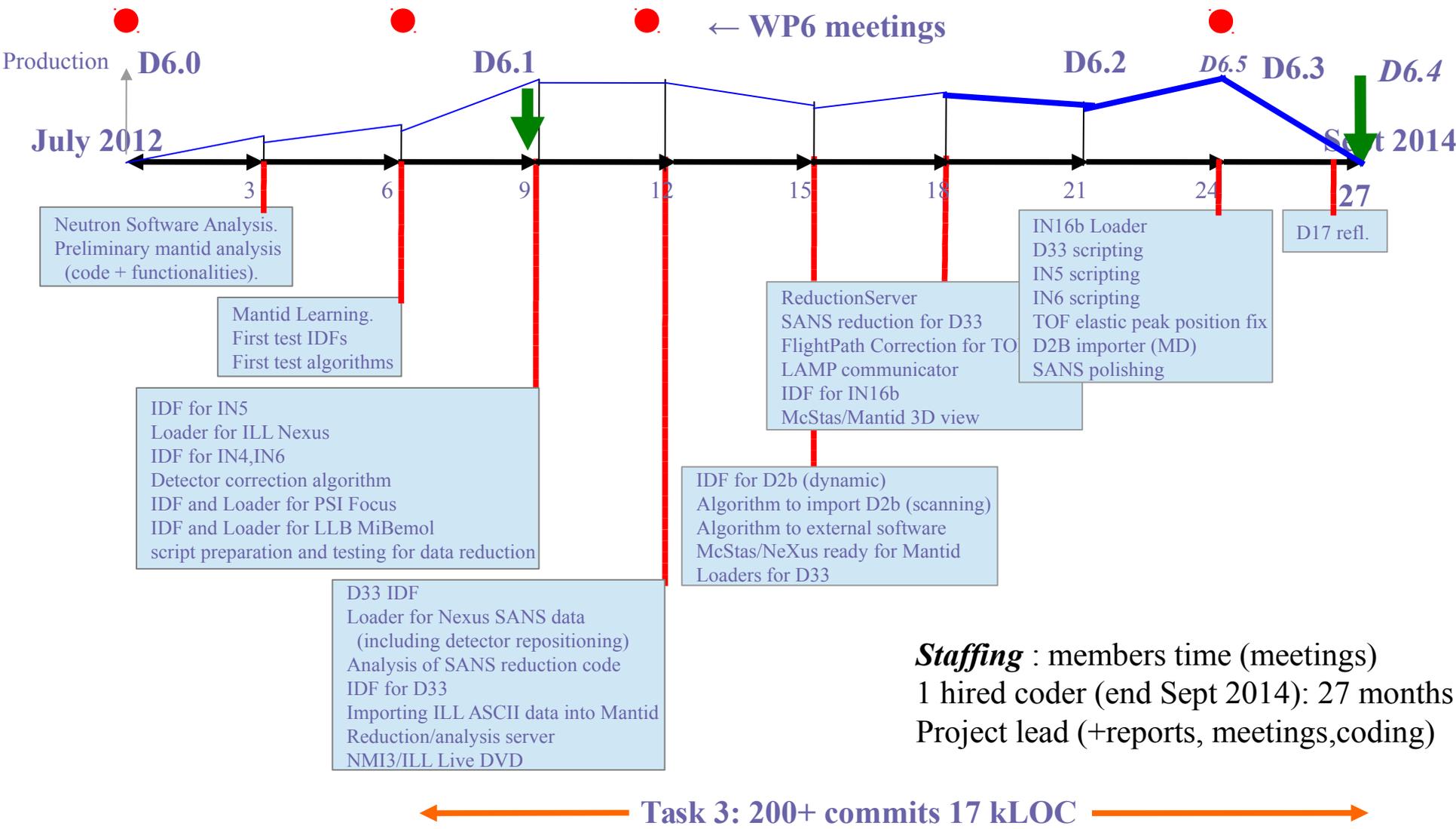
ILL (lead), STFC/ISIS, TUM and JCNS (FRM2), PSI, HZB, CEA LLB,  
HZG/Hamburg, ESS Lund/Copenhagen  
<<http://nmi3.eu/about-nmi3/networking/data-analysis-standards.html>>

## 9 scientific computing groups contributing

**Our tasks: evaluate and facilitate common development  
in reduction/analysis for n/ $\mu$**

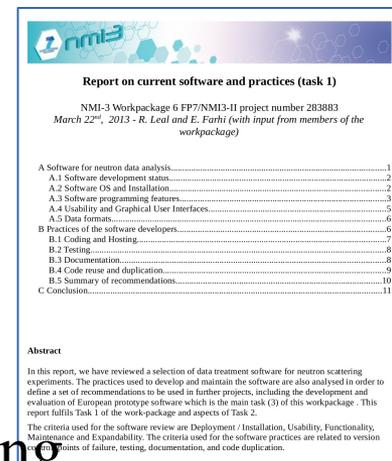
- ✓ Task 1 : Review existing data analysis software and practices of software developers
- ✓ Task 2: Review existing solutions for a common data analysis infrastructure
- ✓ Task 3: Develop prototype software in chosen solution for representative applications
- ✓ Task 4: Evaluate prototype software (*Autumn 2014*)

# WP6 – progress overview



## We have reviewed the current software landscape

- Evaluated 24 software for  $n/\mu$
- Only 5 involve international collaboration
- All active projects (7) use repositories
- Produced a LiveDVD for evaluation/schools
- All recent software use Object Oriented programming
- Active software use mainly : Fortran, C, C++, Matlab, IDL, Python languages, NeXus is spreading
- **Mantid** is today the largest project (by far)



**Report on current software and practices (task 1)**  
NMI-3 Workpackage 6 FP7/NMI3-II project number 283883  
March 22<sup>nd</sup>, 2013 - R. Leal and E. Farhi (with input from members of the workpackage)

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**Abstract**  
In this report, we have reviewed a selection of data treatment software for neutron scattering experiments. The practices used to develop and maintain the software are also analysed in order to define a set of recommendations to be used in further projects, including the development and evaluation of European prototype software which is the main task (3) of this workpackage. This report fulfils Task 1 of the workpackage and aspects of Task 2.  
The criteria used for the software review are Deployment / Installation, Usability, Functionality, Maintenance and Expanding. The criteria used for the software practices are related to version control, points of failure, testing, documentation, and code duplication.

**Recommendations** : Necessity to identify code redundancy and propose **low-level shared libraries** for e.g. models, algorithms, I/O routines, interface design templates.

These should follow adopted **standards**.



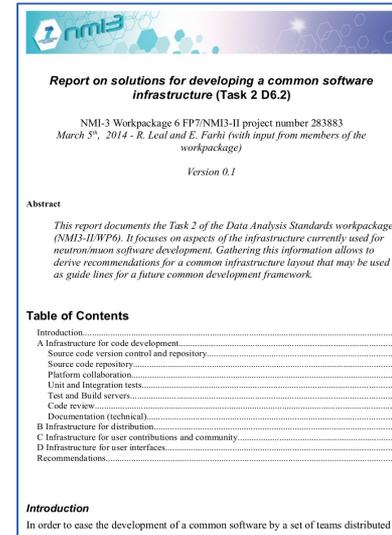
**There is no trend: old software do as good as recent ones**

- What counts is the efficiency, that is the physics/math
- What remains in the end is code that is/can be maintained
- Interoperability could be improved by adopting standards

## We have reviewed infrastructures used for development

- Code location (repository), Collaborative work, Unit testing, Build servers, Code review, Technical documentation
- Software distribution
- User contributions
- Interface homogeneity

**Recommendations:** provide a **community based development infrastructure** with e.g. GIT/SVN, Redmine platform, Jenkins testing/build, Deb/RPM repos, favour **user contributions**.





**Relying on attractive commercial solutions may not be a reasonable solution.**

Prefer community based infrastructure:

- SVN/Git server for storage
- Redmine server for management
- Jenkins build for testing/deployment
- Package repository for distribution



## We have experimented ideas – major WP Task

All code published (github, Mantid, NMI3 web)

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

Mantid contribution available in Mantid release 3.2.1

Helped FRM-II Mantid dev



### Report on the development of prototype software (Task 3 D6.3)

NMI-3 Work-package 6 FP7/NMI3-II project number 283883  
Sept 10<sup>th</sup>, 2014 - R. Leal and E. Farhi (with input from members of the work-package). Version 0.2.

#### Abstract

This report documents the Task 3 of the Data Analysis Standards work-package (NMI3-II/WP6). It details the software that was produced during this project, with code for Mantid and other projects.

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Get a data file (NeXus) → create a 'workspace' (in memory)

Algorithm	Description	Instrument
LoadILL	Loads a ILL nexus file.	<b>ILL: IN4, IN5 and IN6</b>
LoadILLAscii	Loads ILL Raw data in Ascii format.	<b>ILL: D2B</b>
LoadILLIndirect	Loads a ILL/IN16B nexus file.	<b>ILL: IN16B</b>
LoadILLReflectometry	Loads a ILL/D17 nexus file.	<b>ILL: D17</b>
LoadILLSANS	Loads a ILL nexus files for SANS instruments.	<b>ILL: D33</b>
LoadLLB	Loads LLB nexus file.	<b>LLB: MiBemol</b>
LoadSINQFocus → LoadSINQ	Loads a FOCUS nexus file from the PSI	<b>SINQ: FOCUS</b>

In addition: import IN10, IN13, IN16, McStas

Convert workspace(s) into e.g. an other one

<b>Algorithm</b>	<b>Description</b>	<b>Class</b>
CalculateEfficiency	Calculates the detector efficiency for a SANS instrument.	SANS
ConvertEmptyToTof	Converts the channel number to time of flight.	TOF (ILL)
CorrectFlightPaths	Used to correct flight paths in 2D shaped detectors.	TOF (ILL: IN5)
DetectorEfficiencyCorUser	This algorithm calculates the detector efficiency according the formula set in the instrument definition file/parameters.	TOF (ILL: IN4, IN5, IN6)
EQSANSDarkCurrentSubtraction	Perform EQSANS dark current subtraction.	SANS (minor modification)
EQSANSQ2D	Workflow algorithm to process a reduced EQSANS workspace and produce $I(Q_x, Q_y)$ .	SANS (minor modification)

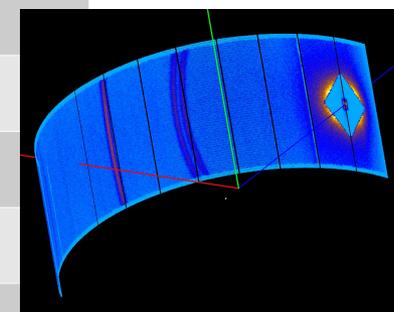
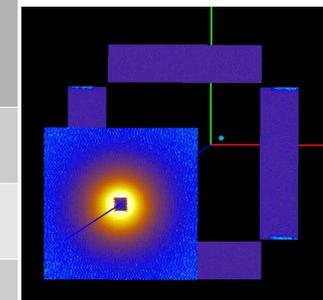
# WP6 – Task 3 – Mantid Algorithms 2

SANSAzimuthalAverage1D	Compute $I(q)$ for reduced SANS data	SANS (minor modification)
SANSBeamFinder	Beam finder workflow algorithm for SANS instruments.	SANS (minor modification)
SANSSensitivityCorrection	Perform SANS sensitivity correction.	SANS (minor modification)
SaveILLCosmosAscii	Saves a 2D workspace to a ascii file usable by COSMOS/LAMP	SANS
SetupILLD33Reduction	Set up ILL D33 SANS reduction options.	SANS (ILL: D33)
TransmissionUtils		SANS (minor modification)
IDF_to_PLY	Convert an IDF into PLY/OFF	Geometry (prototype)

Many other existing algorithms can be used (Sqw, integration, ...)

Describe an instrument detector geometry

File	Description	Has configurable parameters
D2B_Definition	ILL: D2B	
D17_Definition	ILL: D17	Yes
D33_Definition	ILL: D33	Yes
FOCUS_Definition	SINQ: FOCUS	
IN4_Definition	ILL: IN4	Yes
IN5_Definition	ILL: IN5	Yes
IN16_Definition	ILL: IN16	Yes
IN16B_Definition	ILL: IN16B	Yes
MIBEMOL_Definition	LLB: MiBemol	



## Mantid:

- geometry upgrade to allow merge of a set of geometries (for e.g. scan)

## AllToMantid:

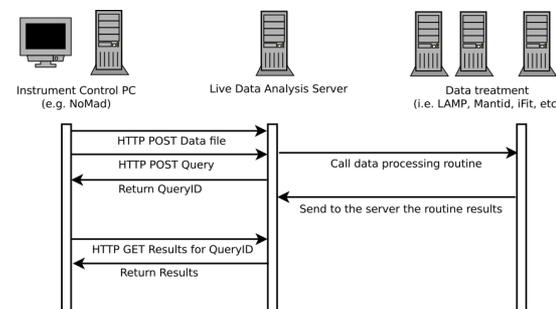
- interface Mantid with any external software by file I/O and pipes.
- Tested with LAMP and iFit.



*iFit*

## ReductionServer:

- a server that gets requests for computational tasks
- distributes them to computational applications, and reports results.



## Evaluation of prototyping when project ends (Sept 2014)

- Support for TOF spectrometers: **functional (powder/liq)**, **no SX**
- Support for SANS: **functional ( $|q|$ )**, **no SX style**
- Support for BackScatt: **mostly functional**
- Support for DIFF: **limited** (not for scanning instruments)
- Support for Reflectometers: **limited** (but improving)
- Support for TAS: **none** (not for scanning instruments)

**Trend** : **Mantid** can handle most, but not all types of experiments. Its **coding effort** is significant. Should be complemented with **other projects** in a coherent way. Currently the only international effort, with NeXus.

## Most coding effort turned towards Mantid



9 importers coded in 2 years → 2+ month/instrument

Use pre-existing Algorithms with minor adjustments when possible.

The SX case (VATES) which was a motivation for the WP6 has not been achieved.

Mantid not adapted to 'scanning' instruments (low-level classes).  
TAS, DIFF (Spin-Echo)

Commit procedure is complex (ticketing and validation)



Same reason to adopt Mantid as to adopt NeXus:

It is an international collaboration  
Good marketing

Today, Mantid represents a major investment for ISIS and SNS.  
Some staff working on it at FRM2, PSI and ILL.

However, it does not prevent to try other solutions, inter-operable, simpler. Some specific topics are missing and may be addressed with alternative solutions (e.g. scans...).



WP6 web site holds the production of the work-package

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

Software, reports, example data files and scripts

Some money left in WP to hold a workshop.

The next EU call 'SINE2020' includes items on data reduction/analysis/simulation.