Data Analysis Standards (WP6)

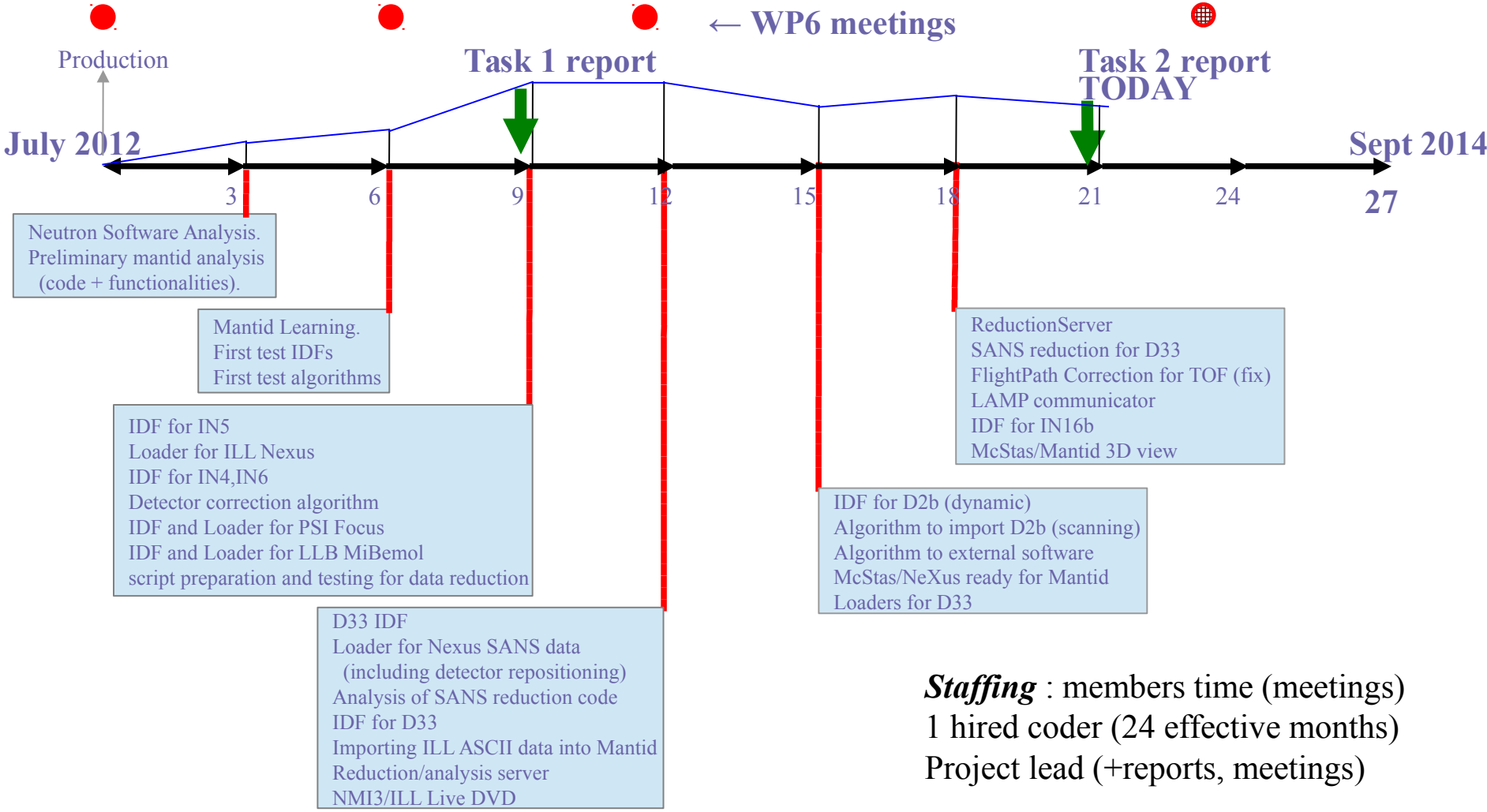
ILL (lead), STFC/ISIS, TUM and JCNS (FRM2), PSI, HZB, CEA LLB, HZG/Hamburg, ESS Lund/Copenhagen
<http://nmi3.eu/about-nmi3/networking/data-analysis-standards.html>

9 scientific computing groups contributing

Our tasks: evaluate and facilitate common development in reduction/analysis for n/μ

- ✔ **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 *(90% done)***
- **Task 4: Evaluate prototype software *(when project ends – Sept 2014)***

WP6 – progress



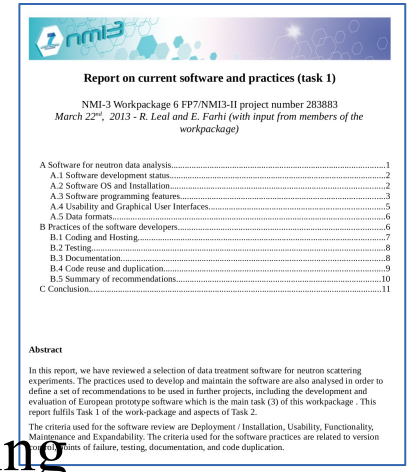
Staffing : members time (meetings)
1 hired coder (24 effective months)
Project lead (+reports, meetings)

Task 3: 166 commits

WP6 – Task 1 – Review software

We have reviewed the current software landscape

- Evaluated 24 software for n/μ
- 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++ and Python languages
- Mantid is today the largest project



Report on current software and practices (task 1)

NMI-3 Workpackage 6 FP7/NMI3-II project number 283883

March 22nd, 2013 - R. Leal and E. Farhi (with input from members of the workpackage)

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 work-package and aspects of Task 2.

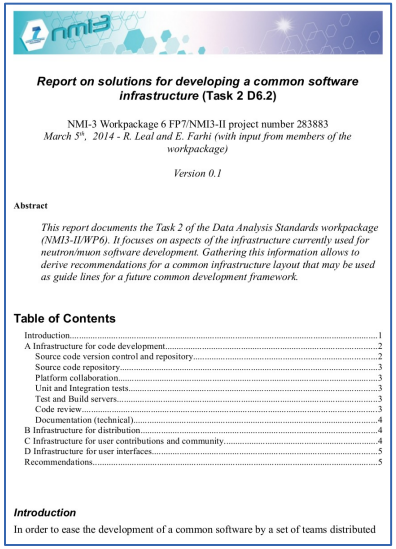
The criteria used for the software review are Deployment / Installation, Usability, Functionality, Maintenance and Expandability. The criteria used for the software practices are related to version control, points of failure, testing, documentation, and code duplication.

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.

WP6 – Task 2 – Infrastructure

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



***Report on solutions for developing a common software infrastructure* (Task 2 D6.2)**

NMI-3 Workpackage 6 FP7/NMI3-II project number 283883
March 5th, 2014 - R. Leal and E. Farhi (with input from members of the workpackage)

Version 0.1

Abstract

This report documents the Task 2 of the Data Analysis Standards workpackage (NMI3-II/WP6). It focuses on aspects of the infrastructure currently used for neutron/muon software development. Gathering this information allows to derive recommendations for a common infrastructure layout that may be used as guide lines for a future common development framework.

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Introduction

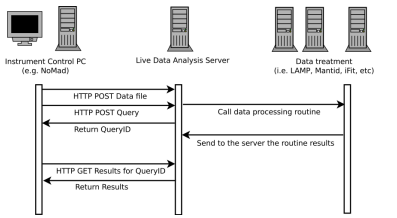
In order to ease the development of a common software by a set of teams distributed

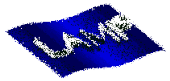
Recommendations: provide a community based development infrastructure at <http://www.neutronsources.org> with GIT/SVN, Redmine platform, Jenkins testing/build, Deb/RPM repos, favour user contributions.

WP6 – Task 3 – Prototype

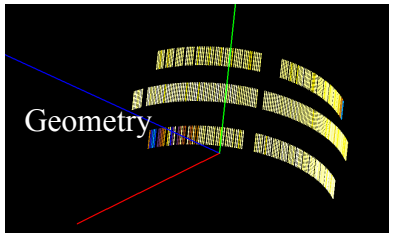
We are experimenting ideas – major WP Task

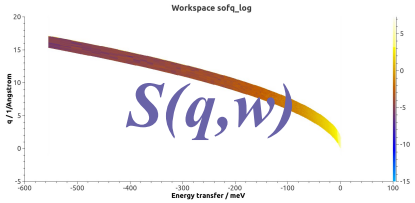
- A 'reduction' server that can execute any task, with any software, and report results.
- A generic algorithm for Mantid that can use external software.
- Importers contributed to the Mantid project, for continuous source instruments and fixes to Algorithms. *IN4-5-6,Focus,MiBemol,D33,D2b,IN16b,McStas*





iFit





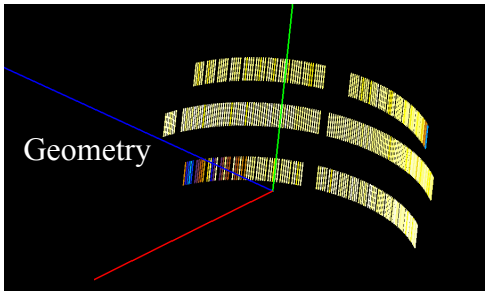
WP6 – Task 3 – Prototype

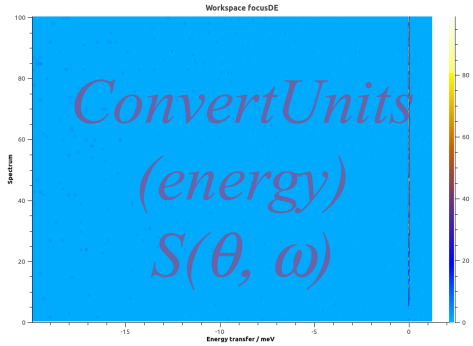
Mantid: PSI Focus (ToF)

Done:

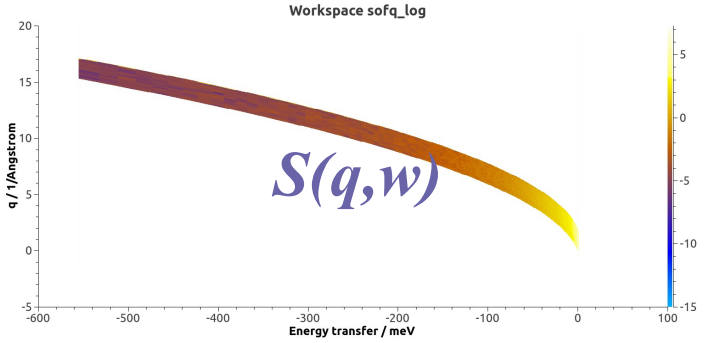
- Instrument geometry (IDF) fixed
- Importer OK
- Corrections for the detector parallax and efficiency OK
- Possibility to use any ToF algorithm, e.g. ConvertUnits, SofQW
- ILL IN4 and IN6
- LLB MiBémol
- PSI Focus

Raw





Reduced



WP6 – Task 3 – Prototype

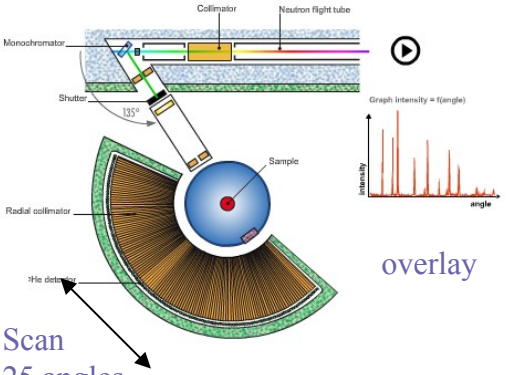
Mantid: ILL D2B (HR powder diffractometer)

Done:

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

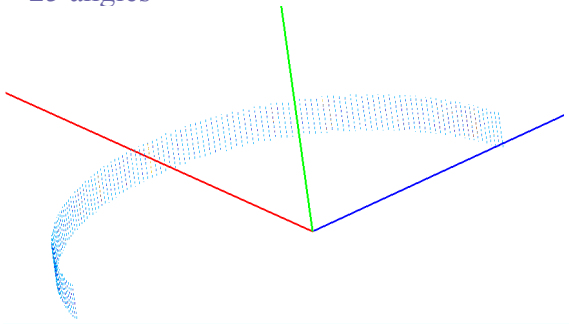
Issues:

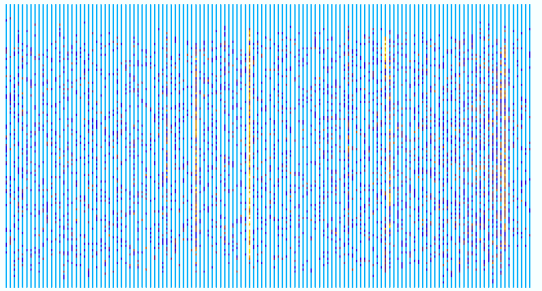
- How to merge different geometries ?
- No detector corrections yet
- Solve this case before switching to e.g. TAS (complex scanning)



overlay

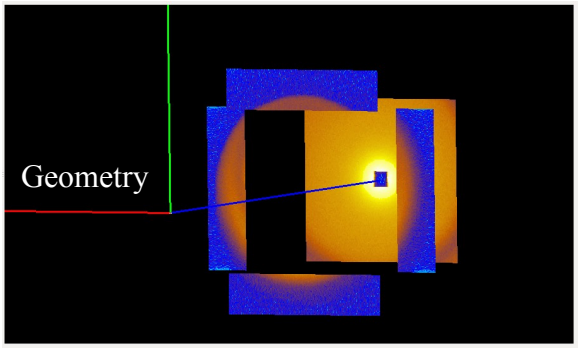
Scan
25 angles

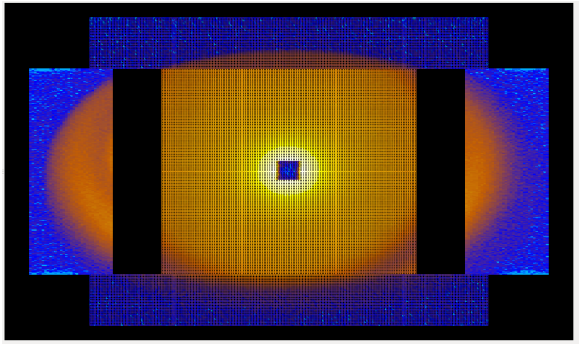




WP6 – Task 3 – Prototype

Mantid: ILL D33 (ToF SANS)





Done:

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

Issues:

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

WP6 – Task 4 – Evaluation

Evaluation of prototyping when project ends

Trend : Mantid can handle most, but not all types of experiments. Its coding effort is significant. Should be complemented by other projects in a coherent way.