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

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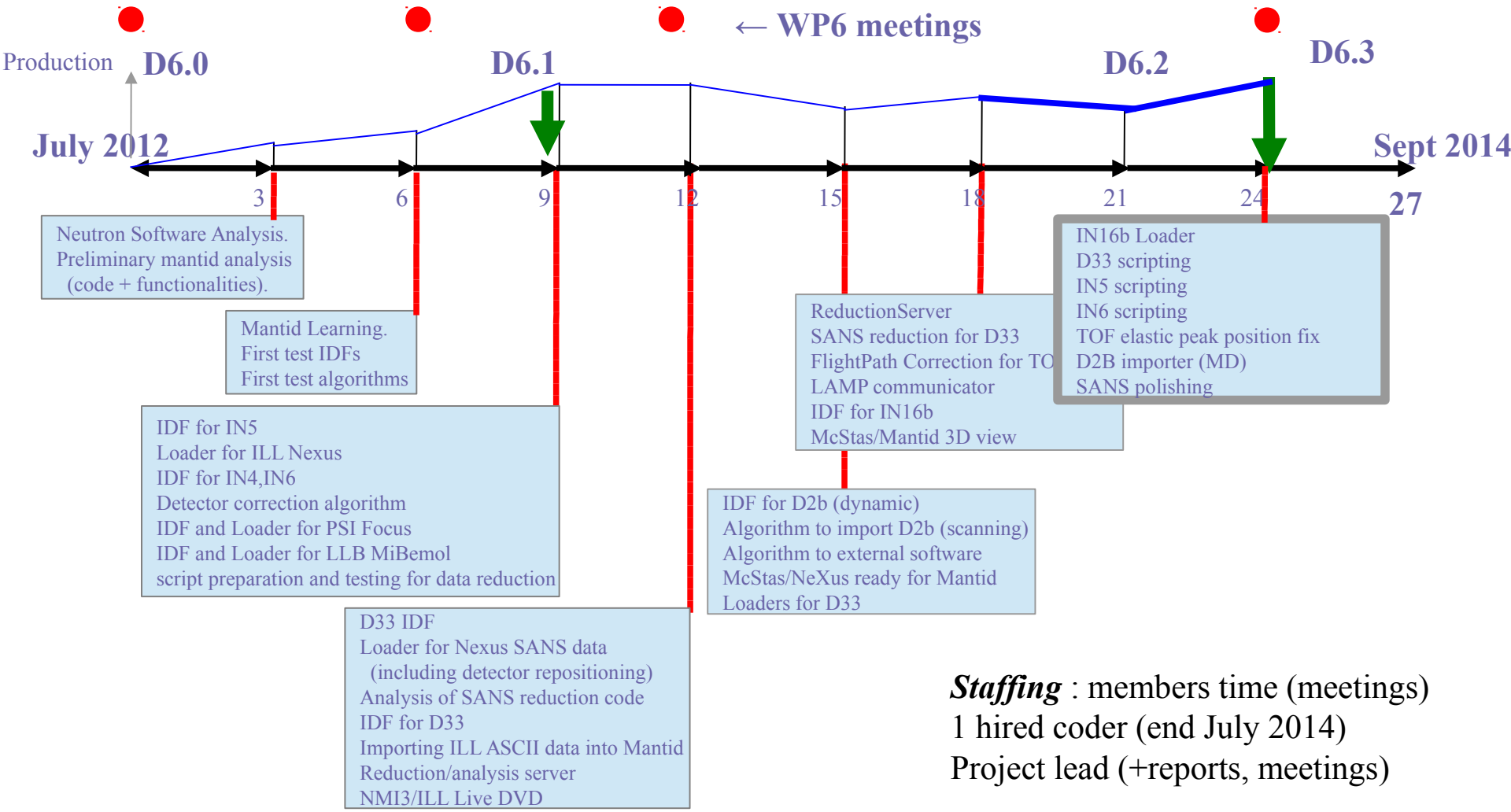
Our tasks: evaluate and facilitate common development in reduction/analysis for n/μ

- ✔ **Task 0 : Testing infrastructure: LiveDVD (June 2012)**
- ✔ **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 *(when project ends – Sept 2014)***
- ✔ **Task 5: Mantid training and user evaluation at the ILL (June 2014)**

WP6 – progress overview



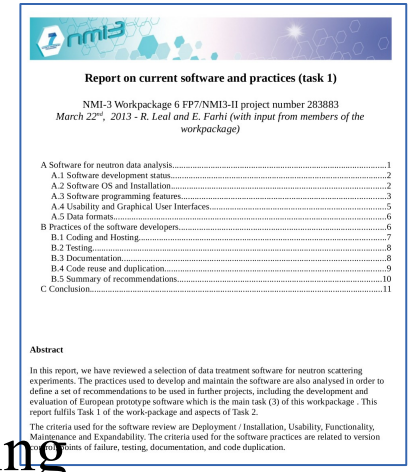
Staffing : members time (meetings)
1 hired coder (end July 2014)
Project lead (+reports, meetings)

Task 3: 200+ 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, NeXus is spreading
- 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)

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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 work-package and aspects of Task 2.

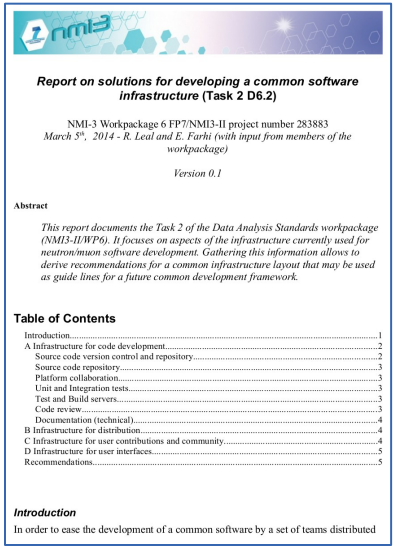
The criteria used for the software review are Deployment / Installation, Usability, Functionality, Maintenance and Expandability. The criteria used for the software practices are related to version control, points of failure, testing, documentation, and code duplication.

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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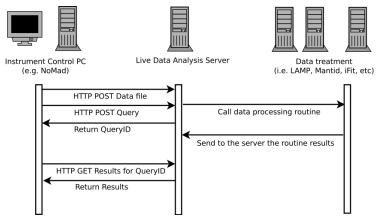
Introduction

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 have experimented 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 ("AllToMantid")
- All code published (github, Mantid, web)
- Importers contributed to the Mantid project, for continuous source instruments and fixes to Algorithms:

IN4-5-6,Focus,MiBemol,D33,D2b,IN16b,McStas,D17
IN10-13-16

Instrument	Example data	Format	Algorithms	Other software
[illegible]	[illegible]N4_064726	nxs	Load (LoadILL) ConvertUnits(Target='DetlaE') procedure [pdf]	LAMP: • rdsum • normalise • in4strip • vnorm • corr_tof • t2e • sqw_rebin
TOF/IN5	Vana: IN5_095893 Data: IN5_096003 Script: IN5_He_4A and its Data.	nxs	Load (LoadILL) ConvertUnits(Target='DetlaE') Rebin SofQW3 CorrectKiKf procedure [pdf]	LAMP: • rdsum • normalise • vnorm • corr_tof • t2e • sqw_rebin
TOF/IN6	Vana Data Script: in6.py and its Data.	nxs	Load (LoadILL) ConvertUnits(Target='DetlaE') Rebin SofQW3 CorrectKiKf procedure [pdf]	LAMP: • rdsum • normalise • vnorm • corr_tof • t2e • sqw_rebin
SANS/D33	D33_041421 D33_041714 Script: process.py and its Data. [illegible] 1422 1425 1427 [illegible] 1431	nxs	Load (LoadILLSANS) SetupILLD33Reduction SANSReduction Rebin SANSAzimuthalAverage1D procedure [html]	LAMP: • rdsum • radial_at
REF/D17	[illegible]7_084347	nxs	Load (LoadILL) [RefLReduction] [REFLReductionInterface] [REFSFReductionInterface]	LAMP: • rdsum • d17_waterdef • d17_waternorm • d17_xyconvert
DIF/D2B	D2B_123944	ascii/INX/NXS	Load (LoadILL) [PowderDiffractionReduction]	LAMP: • rdsum • straight_1d • straight_2d
BS/IN10	IN10_P3OT_350K	ascii/INX/NXS	Load (Indirect_Load_ASCII) Indirect:ConvertToEnergy Indirect:Indirect_Data_Analysis	LAMP: • rdsum • bsnorm • elascan_vnorm • elascan_remov • elascan_slab • elascan_phi2q
BS/IN13		ascii/INX/NXS	Load (Indirect_Load_ASCII) Indirect:ConvertToEnergy	LAMP: • rdsum • bsnorm • in13_elascan_v

WP6 – Task 4 – Evaluation

Evaluation of prototyping when project ends (Sept 2014)

Support for TOF spectrometers: functional
Support for SANS: functional
Support for BackScatt: mostly functional
Support for DIFF: limited (not for scanning instruments)
Support for Reflectometers: limited
Support for TAS: none (not for scanning instruments)

Full code and reports available (web, github, Mantid commit)

Future of WP6: probably 1-2 further meetings possible, no dev.

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.
Currently the only international effort, with NeXus.