

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*)



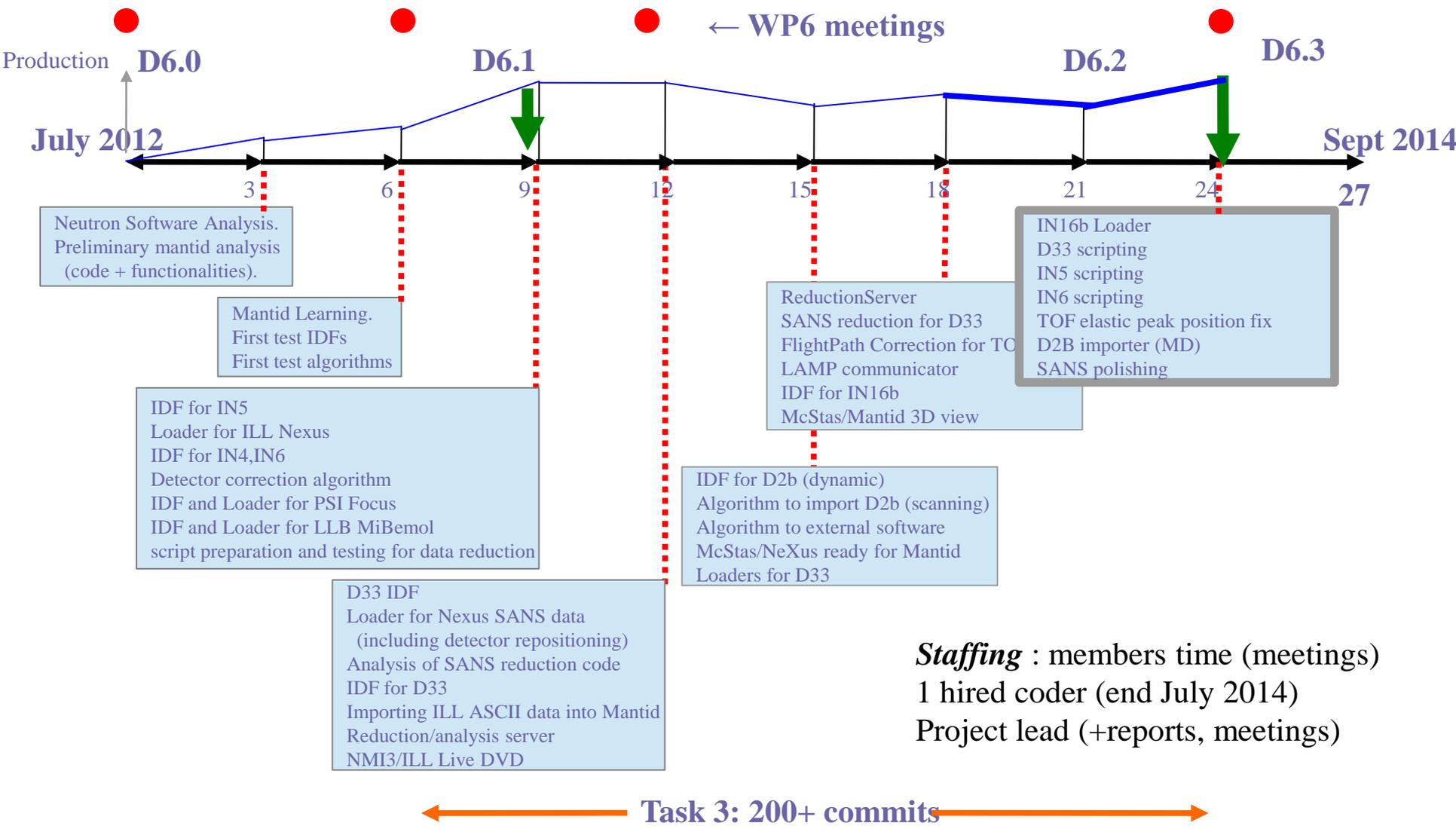
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- ✓ **Task 0 : Testing infrastructure: LiveDVD (June 2012)**
- ✓ **Task 1 : Review existing data analysis software and practices of software developers**
- ✓ **Task 2: Review existing solutions for a common data analysis infrastructure**
- ✓ **Task 3: Develop prototype software in chosen solution for representative applications**
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- ✓ **Task 5: Mantid training and user evaluation at the ILL (June 2014)**

WP6 – progress overview



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 get a set of recommendations to be used in further projects, including the development and evaluation of European prototype software which is the main task (2) 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.

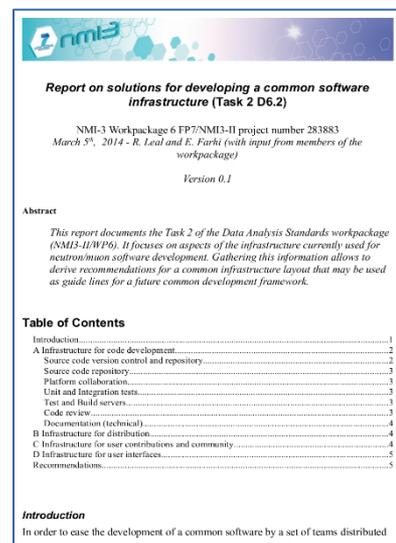
Recommendations : Necessity to identify code redundancy and propose **low-level shared libraries** for e.g. models, algorithms, I/O routines, interface design templates.

These should follow adopted **standards**.



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** at <http://www.neutronsources.org> with GIT/SVN, Redmine platform, Jenkins testing/build, Deb/RPM repos, favour **user contributions**.

We have experimented ideas – major WP Task

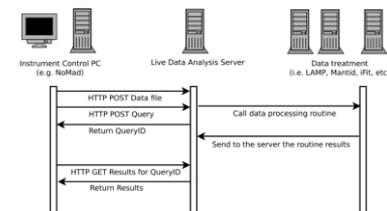
- A 'reduction' server that can execute any task, with any software, and report results.

- 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
IN4-5-6	Vana: IN4_064726	ISIS	Load (LoadILL) ConvertUnits(Target=DataE) procedure [pdf]	LAMP: • rdsun • normalise • loadstrip • vnorm • corr_tof • l2e • sqw_rebin
TOF/IN5	Vana: IN5_095893 Data: IN5_096003 Script: IN5_He_4A and its Data	ISIS	Load (LoadILL) ConvertUnits(Target=DataE) Rebin SoftQW3 CorrectKIKI procedure [pdf]	LAMP: • rdsun • normalise • vnorm • corr_tof • l2e • sqw_rebin
TOF/IN6	Vana Data Script: In6.py and its Data.	ISIS	Load (LoadILL) ConvertUnits(Target=DataE) Rebin SoftQW3 CorrectKIKI procedure [pdf]	LAMP: • rdsun • normalise • vnorm • corr_tof • l2e • sqw_rebin
SANS/D33	D33_041421 D33_041714 Script: process.py and its Data. 1422 1423 1427 1431	ISIS	Load (LoadILLSANS) SetupLLLD33Reduction SANSReduction Rebin SANSAzimuthalAverageID procedure [html]	LAMP: • rdsun • radial_at
REF/D17	D17_084347	ISIS	Load (LoadILL) [RefLLReduction] [RFFSReductionInterface] [RFFSReductionInterface]	LAMP: • rdsun • d17_waterdif • d17_waternorm • d17_xyconvert
DIF/D2B	D2B_123944	ascii/INXNNS	Load (LoadILL) [PowderDiffractionReduction]	LAMP: • rdsun • straight_1d • straight_2d
BS/IN10	IN10_P30T_350K	ascii/INXNNS	Load (Indirect_Load_ASCII) Indirect.ConvertToEnergy Indirect.Indirect_Data_Analysis	LAMP: • rdsun • detnorm • eliscan_vnorm • eliscan_remove • eliscan_slab • eliscan_ph02g
BS/IN13		ascii/INXNNS	Load (Indirect_Load_ASCII) Indirect.ConvertToEnergy	LAMP: • rdsun • detnorm • ml3_eliscan_v



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.