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

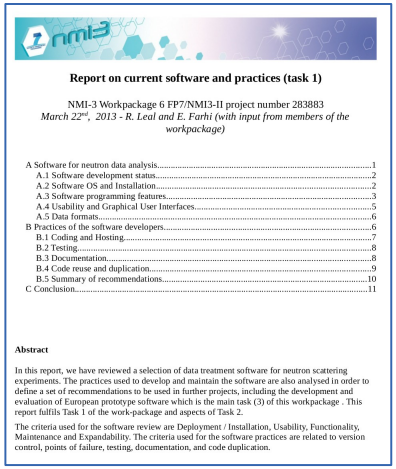
27 months funding

- ✔ **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**

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++, 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 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 1 – Comments

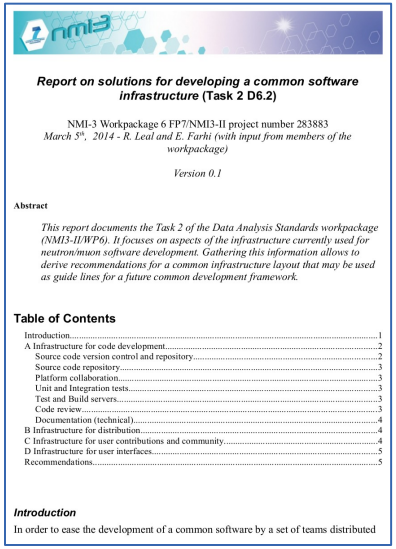
There is no trend: old software do as good as recent ones

- 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

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 with e.g. GIT/SVN, Redmine platform, Jenkins testing/build, Deb/RPM repos, favour user contributions.

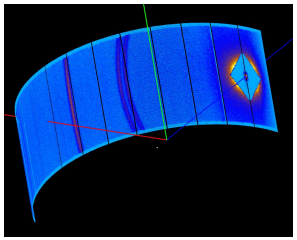
WP6 – Task 3 – Prototype

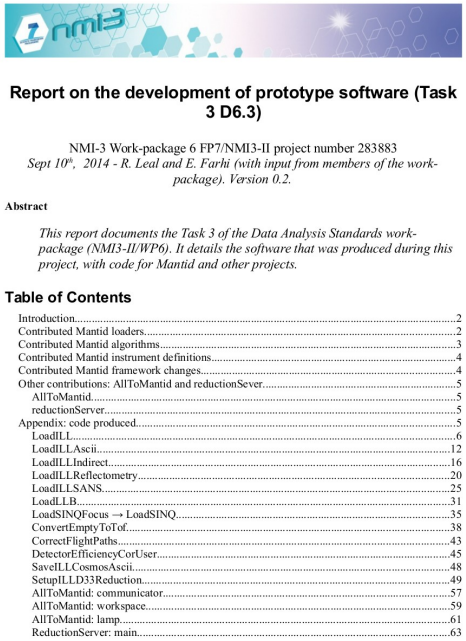
Constitutes the major WP Task

- All code published (github, Mantid, NMI3 web)

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

- Mantid contribution available from Mantid 3.2.1
- Loaders: 7 ILL instruments, 1 LLB, 1 PSI
- Algorithms: 6 (reduction)
- Geometries: 9 (detectors)
- All pushed into Mantid





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

NMI-3 Work-package 6 FP7/NMI3-II project number 283883
Sept 10th, 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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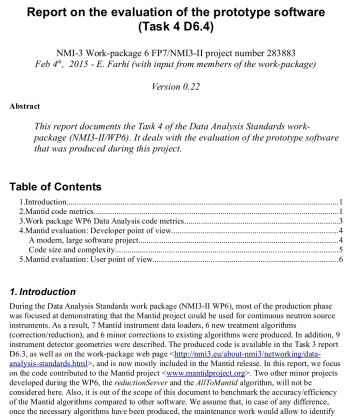
WP6 – Task 4 – Evaluation

Evaluation of our prototyping at project ends (Jul'12- Sept'14)

Support for TOF spectrometers: functional (powder/liq)
Support for SANS: functional ($|q|$)
Support for BackScatt: mostly functional
Support for DIFF: limited at reactors (not for moving)
Support for Reflectometers: limited (but improving)
Support for TAS: none (these really move...)



Report on the evaluation of the prototype software (Task 4 D6.4)

NMI-3 Work-package 6 FP7/NMI3-II project number 283883
Feb 4th, 2015 - E. Farhi (with input from members of the work-package)

Version 0.22

Abstract

This report documents the Task 4 of the Data Analysis Standards work-package (NMI3-II/WP6). It deals with the evaluation of the prototype software that was produced during this project.

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1. Introduction

During the Data Analysis Standards work package (NMI3-II WP6), most of the production phase was focused at demonstrating that the Mantid project could be used for continuous neutron source instruments. As a result, 7 Mantid instrument data loaders, 6 new treatment algorithms (correction/reduction), and 6 minor corrections to existing algorithms were produced. In addition, 9 instrument detector geometries were described. The produced code is available in the Task 3 report D6.3, as well as on the work-package web page <http://nmi3.eu/about-nmi3/networking/data-analysis-standards.html>, and is now mostly included in the Mantid release. In this report, we focus on the code contributed to the Mantid project <www.mantidproject.org>. Two other minor projects developed during the WP6, the *reductionServer* and the *AllToMantid* algorithm, will not be considered here. Also, it is out of the scope of this document to benchmark the accuracy/efficiency of the Mantid algorithms compared to other software. We assume that, in case of any difference, once the necessary algorithms have been produced, the maintenance work would allow to identify

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

WP6 – Task 4 – Comments

Most coding effort turned towards Mantid

15 'algorithms' coded in 2 pers.years
Use pre-existing Algorithms with minor adjustments when possible.

The SX case (VATES) which was a motivation for the WP6 has not been achieved in WP6, but progresses at ISIS/SNS.

Mantid not yet adapted to 'moving' instruments.
e.g. TAS, 'reactor' DIFF

Mantid is a large project.
Maintenance requires permanent dedicated staff.

WP6 – Why Mantid ?

Same reason to adopt Mantid as to adopt NeXus:

It is an international collaboration
Good marketing
A unique software across neutron facilities

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

Success ensured with proper funding.

Some specific topics are missing and may be addressed with alternative solutions (e.g. scans...).

WP6 – Outcome of WP6

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

Most technical contributions part of Mantid

The 'SINE2020' includes items on
data reduction/analysis/simulation/e-learning.