

1. Publishable summary

The Data Analysis Standards work-package (WP6) is a networking activity which aims at determining how to develop, deploy and operate a common data analysis software infrastructure to facilitate joint software development for the neutron scattering and muon community in Europe. An analysis of the existing software landscape and coding practices is the starting point of this activity. Then, a limited set of data treatment functionalities will be implemented in an inter-facility common infrastructure, demonstrating the applicability of high-end coding standards. As part of this effort, a set of recommendations for coding software, as well as for project management at the level of an EU common software infrastructure for neutron/muon facilities, will be proposed. This way, we wish to motivate scientist programmers to adopt common standards in order to favour software interoperability and collaboration.

2. Project objectives for the period

2.1 Project objectives

High resolution detectors and higher data rates, among others, make new demands on software that require professional software solutions. In particular, new instruments constitute a considerable challenge for software provision and failure to address this issue leads to a delay in the scientific impact of new investment.

The importance of data analysis has now become clear and is becoming a focal point of efforts to optimise scientific production.

The aim of this networking activity is to determine how to develop, deploy and operate a common data analysis software infrastructure to facilitate joint software development in the neutron scattering community.

The Data Analysis Standards networking work-package (WP6) will begin with two review tasks: review existing data analysis software and practices of software developers and review existing solutions for a common data analysis infrastructure. Based on the reports from these tasks, the key phase of the project will be to develop a small number of prototype software solutions in areas chosen by the partners. The goal will be to deploy functionality that exists at some facilities in the common framework thereby making it accessible to and optimised for all partners.

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

2.2 Work progress and achievements

The work package started in June 2012 with the recruit of a trained staff.

In order to ease the evaluation step of the project, a set of easily available software for neutrons and muons science was identified and gathered into a Live DVD, that is an operating system holding on a DVD, that can be used without affecting the computer content. This DVD can be used on any current computer to evaluate the pre-installed software, as well as during workshops, tutorials and training sessions. It can be obtained from <<http://nmi3.eu/about-nmi3/other-collaborations/data-analysis-standards.html>>. This task, which was not initially in the list of deliverables, required about a month.

The evaluation of current software revealed a sparse landscape which is substantially far from the definition of standards. Consequently, handling this diversity required longer than expected. In parallel to this task, getting acquainted with the Mantid project, which is to be evaluated as part of this work-package, required about 6 months. However, learning about Mantid was considered essential before the task 1 of the project could be achieved. For these reasons, the “Report on current software and practices” (task 1 deliverable)

was produced after its planned date. The Task 1 report, which was published in March 2013 after approval and input from the work-package members, has been published on our project page. It consists in an analysis of 24 existing and easily available software packages. The programming methodologies, user experience, data formats, as well as current practices are detailed. A list of recommendations is then produced.

The Task 2, which aims at reviewing current practices for a common data analysis infrastructure, mainly deals with technical aspects needed to organise a large software project. These aspects are partly discussed in the Task 1 report. Even though the associated report has not been delivered yet, this ongoing task is well advanced, to be completed by Autumn 2013. We are considering both the technical aspects (repositories, documentation, ...), as well as organizational aspects (project management).

The 3rd Task, which constitutes to core of the work-package, is progressing fast, with a strong implication into the Mantid project. To date, six continuous source based instrument data set importers for Mantid have been produced (IN4, IN5, IN6, D33 at the ILL, MiBemol at the LLB, and Focus at the PSI). The existing Mantid 'algorithms' for data reduction have then been applied and compared with equivalent 'macros' in LAMP. It was found that in some cases Mantid is faster than LAMP (loading data), and in some others slower. Also, Mantid requires significantly more memory to store data sets than LAMP, as the time axis is duplicated for all pixels composing the detectors, whereas some other packages (e.g. LAMP) prefer a unique definition shared by all detector pixels. All in all, we find that results from Mantid and LAMP compare well.

The Task 4 requires Task 3 to be completed, and will thus only start by the end of the project.

Actually, the work-package will provide a clearer view about the existing software landscape for neutron/muon scattering, and the methodologies that have been used to produce these tools. Our contribution to the Mantid project is part of an evaluation, but will however bring a set of algorithms dedicated to continuous neutron source instruments. We hope that this contribution will be used by the community, either from Mantid itself, or as a component in other software. Finally, we wish to produce a list of recommendations for coding standards and methodologies, that could ease the future development of inter-facility software.

3. Deliverables

DELIVERABLES									
Del. no.	Deliverable name	WP no.	Lead beneficiary	Nature	Dissemination level	Delivery date from Annex I (proj month)	Actual / Forecast delivery date	Delivered Yes/ No/ Ongoing	Comments
D6.0	Catalogue of existing software	6	ILL	other	public	-	1	Yes	New deliverable as a DVD on <nmi3.eu> website
D6.1	Report on current software and practices	6	ILL	report	public	2	10	Yes	Late staff recruit, longer than expected training period.
D6.2	Report on solutions for developing a common software infrastructure.	6	ILL	report	public	4	15	Ongoing	Late staff recruit, longer than expected training period.
D6.3	Prototype software in chosen solution	6	ILL	prototype	public	18	20	Ongoing	Part of <mantidproject.org>
D6.4	Report on evaluation of prototype software.	6	ILL	report	public	24	27	Waiting	Wait for completion of D6.3