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Working Material

Data Acquisition & Analysis for Neutron Beam Line Experiments

Report of a Consultancy Meeting

IAEA, Vienna, Austria, 10-12 December 2008

Reproduced by the IAEA

Vienna, Austria, January 2009

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1. FOREWORD

The IAEA promotes networking and regional collaboration to improve the efficient utilization of research reactors (RRs). Currently there are more than 240 operational RRs world wide, and over 100 have a thermal power greater to or equal to 1 MW. This provides the potential for effective neutron beam applications. Many well known RRs are over booked, receiving nearly 3 times more experimental proposals than available beam time. This situation could be considerably improved if, in addition to other various measures, **standardization of data acquisition, protocol formats, soft- and hardware-interfaces and data analysis procedures** were developed and implemented. This would allow more efficient share and use of the beam time, facilitate multi-facility access for external users, make much more flexible on-line & off-line data analysis including interpretation of results. Some instrumentation development, tests and calibration measurements could be successfully performed in less “busy” RR facilities thanks to the commonly accepted data formats and analysis procedures. All that would encourage further development and more efficient use of neutron beam lines in the developing Member States, while at the same time improving the performance and accessibility of overbooked facilities.

A good example of such efforts is seen already within the STRAINET network (in collaboration with the IAEA), where material residual stress and texture analysis for industrial applications are performed using common formats and interfaces. The development, validation and harmonization of techniques, procedures and tools are done within the international co-operation, where all partners agree on the unified approach to be shared and adopted among them. Indeed, the well accepted and standardized data formats, common analysis procedures and interpretation of results ensure a fast and flexible response to the requirements of industrial partners being the end users in this particular case.

This Consultancy Meeting was attended by 6 international experts from Europe (2), Asia (1), Pacific (1), USA (1), Africa (1), and chaired by Mr. Richard Riedel. The major drafting of the report was done by Mr. Rainer Schneider. Mr. Oliver Kirstein from ANSTO attended the meeting at cost-free for the Agency. The IAEA officer responsible for this document is Mr. Danas Ridikas of the Physics Section, Division of Physical and Chemical Sciences, Department of Nuclear Sciences and Applications. The meeting was held at the IAEA, Vienna, Austria.

2. EXECUTIVE SUMMARY

The meeting participants felt it important to provide the following general remarks before formulating the recommendations:

In order to promote international co-operation and knowledge dissemination in the field of neutron research, it is important to encourage and establish “standardization of interfaces”. Such measures would facilitate efficient international networking activities especially by avoiding redundancies. Besides local mechanic and electronic hardware that is very expensive to be standardized (exchanged) at the neutron facilities, the definition of standards for software interfaces as well as data formats can play the key role to initiate/enlarge international collaboration and data exchange in this field. If common standards were implemented, both new upcoming neutron sources from the developing countries as well as the established neutron facilities would profit strongly from such projects.

The meeting experts recommended that the actions should be taken to:

- Encourage and assist new neutron beam applications in the use of data format based on NeXus (as a recommended standard). This could be realized within the pilot project related to the residual stress measurements (STRAINET);

- Facilitate and support fellowship program for international exchange and training (e.g. researchers from emerging new facilities will be hosted by the established facilities for the training both in hardware and software for neutron beam applications).
  Potential fellowship projects might be:
  a) Review of current best practices driven by new developments at emerging and established facilities used to lever common trends and evolve standards related to modularity. The Agency should try to encourage new projects to work along and implement the defined standards.
  b) Realization of well-defined modules using standard communication interfaces as web services (e.g. local sample environment: high-temperature furnace on the powder diffraction instrument) in order to facilitate international cooperation and standardization;

- Assist in establishment of a data base on data acquisition and analysis for neutron beam applications hosted and managed at the IAEA; facilitate the transfer of information about related meetings (NIAC, NOBUGS) on a dedicated web-page and support the participation from the developing member states

- Encourage and support established topical DAS conferences to be organized at the facilities in the developing countries with new neutron beam projects; a dedicated session on data acquisition and analysis systems for neutron beams might be organized in during the coming RR conference in 2011

- Actively participate in promoting the use of neutron beam experiments through virtual experiments, assist in creation and promotion of a toolkit for the production of numerical data using McStas description of instruments at existing facilities (e.g. in this way training for data analysis based on numerical data could be achieved/promoted/explained before the real experiment takes place).

3. OBJECTIVES OF THE MEETING

Use of neutron beam techniques employed at research reactors (RRs) is central for advances in basic research as well as for a number of applications including energy sector. The common approach for unification and standardization of data acquisition, data handling and analysis, interpretation of experimental results is of great importance for all Member States being involved in neutron beam experiments. Indeed, the demand from developing countries on learning/adopting data acquisition and analysis systems used at well established neutron beam facilities remains substantial. In this context, the proposed consultancy meeting aimed to identify and recommend certain neutron beam applications, where **harmonization and standardization of data acquisition and analysis systems** is desirable and practically feasible/achievable. In the future, further initiatives could be made in terms of Technical Meetings, CRPs, or thematic ICTP workshops, so these recommendations could be successfully implemented (e.g. through the user networks, national or regional technical cooperation projects, bilateral collaborations, fellowships, exchange of scientists and students, etc.).

The specific objectives of the proposed meeting are:

- Identify and characterize the needs on unification and standardization of data acquisition and analysis for neutron beam line experiments (e.g. neutron scattering experiments, residual stress measurements, neutron radiography, etc.)
- Suggest neutron beam applications, where RR user networks could be initiated in relation with harmonization and standardization of data acquisition and analysis
- Outline the breakthroughs in R&D on data acquisition and analysis systems in emerging neutron beam applications as Quasi-Laue Diffraction, Ultra-SANS, 3D Neutron Tomography, etc.
- Evaluate the role RRs can play in development and testing of dedicated data acquisition and analysis systems to be used in new generation spallation neutron sources.

4. BACKGROUND SITUATION ANALYSIS

4.1. Expectations and Requirements for Common Standard Data Formats and Software Interfaces

The following points summarize the discussions on expectations and requirements for standards of data formats and data software interfaces:

- The data format should be flexible in order to cover the requirements for the wide range of possible neutron scattering instruments, sample environment equipment and sample manipulation setups (hexapod, robot arm, digital cameras, etc.)
- There should be easy-to-use routines for data input and output for different software development platforms
- There should be no restrictions concerning real-time data and huge data sets that are emerging at state-of-the-art time-of-flight setups or tomography stations. Binary data formats would be preferable in order to enable fast data in/output
- The experimental data/protocol files should contain the complete available set of raw data without information reduction together with all information about calibration and instrument setup parameters. At least a link to the data, valid for the experiment, must be set
- The data format should assist in the economic use of the instrument (reliability, repeatability and possibility to share of the experimental results)

Today NeXus is the only data format that can be looked upon as an international accepted standard. The structure of NeXus files is extremely flexible. It can accommodate very complex instrumental information, if required, but it can also be used to store very simple data sets. Therefore the authors recommend the use of this data format.

4.2. The NeXus Format

4.2.1 Introduction

NeXus is becoming a common data format for neutron, x-ray, and muon science. It is being developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data and is managed through the NIAC committee.

In recent years, a number of scientists and computer programmers working in neutron and synchrotron light facilities around the world came to the conclusion that a common data format would fulfill a valuable function in the scattering community. As instrumentation becomes more complex and data visualization become more challenging, individual scientists or even institutions have found it difficult to keep up with new developments on the local basis only. A common data format makes it easier, both to exchange experimental results and to exchange ideas about how to analyze them. It promotes greater cooperation in software development and stimulates the design of more sophisticated visualization tools. (*Source:* *www.nexusformat.org*)

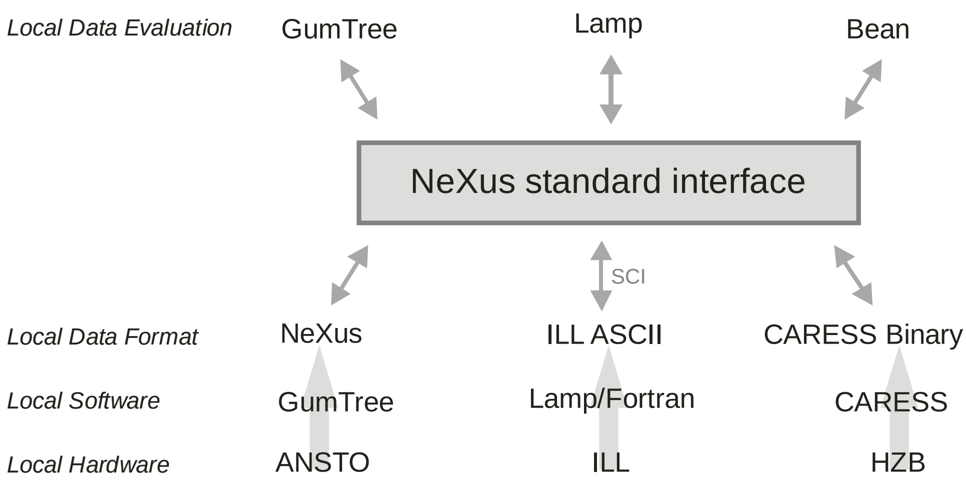


***Figure 1:*”Nexus as currency”**: *A common data format introduces an artificial interface layer that allows the exchange of experimental results. Here a schematic representation is shown for the neutron facilities ANSTO, ILL and HZB, all able to “communicate” thanks to Nexus.*

4.2.2 The structure of the NeXus data format

In brief, NeXus data formats have four components:

1) a set of subroutines to make it easy to read and write NeXus files,
2) a set of design principles to help people understand what is in them,
3) a set of instrument definitions to allow the development of more portable analysis software, and
4) a set of low-level file formats to actually store NeXus files on physical media.

A Set of Subroutines

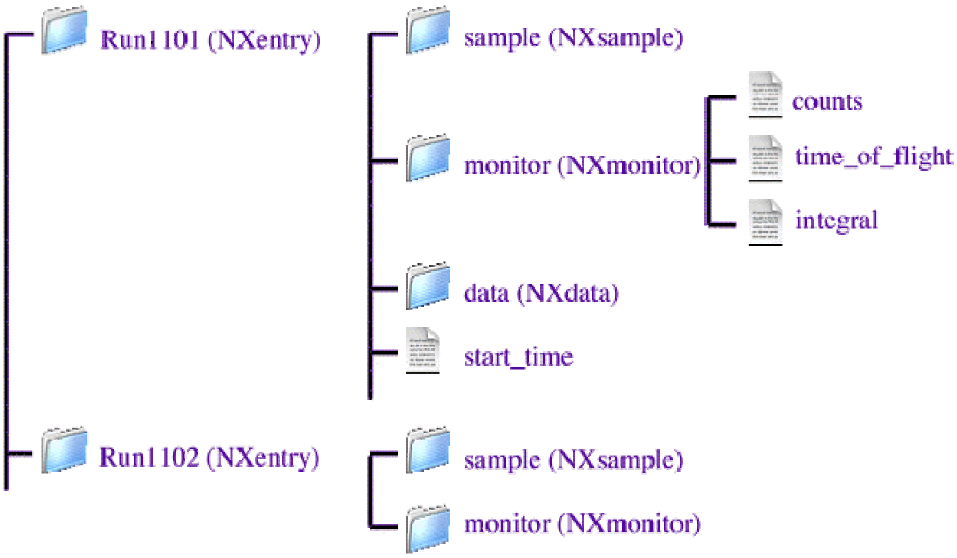
In the past, a data format was defined by a document describing the precise location of every item in the data file, either as row and column numbers in an ASCII file, or as record and byte numbers in a binary file. In modern data formats, such as NeXus, the user does not need to know where the data are stored. Instead, the user should be aware of the names/attributes, how these data are called. It is the job of the subroutine library to retrieve the data afterwards.

A Set of Design Principles

NeXus data files contain two types of entity: data items and data groups. Data Items can be scalar values or multidimensional arrays of a variety of sizes (1-byte, 2-byte, 4-byte, 8-byte) and types (characters, integers, floats). Extra information required to describe a particular data item, such as the data units, can be stored as a data attribute. Data Groups are like folders that can contain a number of data items and/or other groups. In fact, a NeXus file can be viewed as a computer file system. Just as files are stored in folders (or subdirectories) to make them easy to locate, so NeXus data items are stored in groups. The group hierarchy is designed to make it easy to navigate inside the NeXus data file.

Example of a NeXus File

The following diagram shows an example of a NeXus file represented as a tree structure.



Important Classes

Here are some of the important classes found in nearly all NeXus files. A complete list can be found in the NeXus Design page.

> *NXentry:* The top level of any NeXus file contains one or more groups with the class NXentry. These contain all the data that is required to describe an experimental run or scan. Each NXentry typically contains a number of groups describing sample information (class NXsample), instrument details (class NXinstrument), and monitor counts (class NXmonitor).
>
> *NXdata:* Each NXentry group contains one or more groups with class NXdata. These groups contain the experimental results in a self-contained way, i.e., it should be possible to generate a sensible plot of the

data from the information contained in each NXdata group. That means it should contain the axis labels and titles as well as the data.

NXsample: A NXentry group will often contain a group with class NXsample. This group contains information pertaining to the sample, such as its chemical composition, mass, and environment variables (temperature, pressure, magnetic field, etc.).

NXinstrument: There might also be a group with class NXinstrument. This is designed to encapsulate all the instrumental information that might be relevant to a measurement, such as flight paths, collimations, chopper frequencies, etc.

Since an instrument can comprise several beam-line components each defined by several parameters, they are each specified by a separate group. This hides the complexity from generic file browsers but, at the same time, makes the information available in an intuitively obvious way if it is required.

A Set of Instrument Definitions

If the design principles are followed, it will be easy for anyone browsing a NeXus file to understand what it contains, without any prior information. However, if you are writing visualization or analysis software, you will need to know precisely what information is contained in advance. For that reason, NeXus provides a way of defining the format for particular instrument types, e.g., time-of-flight small angle neutron scattering. This requires some agreement by the relevant communities, but would allow the development of much more portable software. These instrument definitions are being formalized as XML files, using a specially devised syntax that specifies the names of data items, and whether they are optional or required. The following is an example of such a file for the simple NeXus file shown above.

A Set of Low-Level File Formats

To actually store NeXus files on physical media, different low-level file formats are available, namely HDF4, HDF5, and XML. The NeXus library may be configured to support all of them, or any non-empty subset. Applications that create NeXus files need to decide (or let the user decide) in which low-level format data shall be stored. Generic data analysis applications should be able to read any low-level format. (*Source:* *www.nexusformat.org*)

4.2.3 Recommendations

- Fast establishment of NeXus compatibility at all neutron facilities. For the realisation of the NeXus data format at the different neutron facilities there are two possibilities. First and most simple: The data format written by the remote control software should be done according the NeXus conventions. Second and less desired: If not possible a pre-NeXus format can be used to be translated into NeXus afterwards. New facilities should use the NeXus data format from the beginning.

- For each type of instruments an instrument class has to be defined. Any community is invited to define the “standard” of their instruments. The instrument definition should be done by one key player of the community trying to optimize overlap between existing NeXus implementations for these types of instruments. Pilot Projects: Standardization of the NeXus format for StrainScanning community (STRAINET). HZB intends to propose a draft NeXus format for StrainScanners developed for StressSpec at FRM-II. The neutron tomography community should work along the same ideas. Minimum requirements for the NeXuS format should be defined at the very beginning, while complete experiment information can be added later.

- The neutron community should be aware of the developments at the NIAC committee, and it is the role of NIAC to disseminate the information.

4.3. Recommendations for Remote Control / Data Analysis Software

In order to prevent bottlenecks and to facilitate sharing of software, the NeXus compatibility is of enormous importance. Additional standardized interfaces within modularized remote control / data analysis software frameworks could help to avoid unnecessary duplication of software developments as well. The discussions during the meeting resulted in a recommendation of a "nugget-like" plug-in structure that enables network developments based on Web services. Nuggets will enable new functionality to the instrument control software, even in the command language. They can be used for "slow" controls only. In this regard, exceptional handling has to be developed. The nuggets are ideal for user in-situ equipment, remote control of LabView-type controlled hardware. Mathlab can be used that way, too.

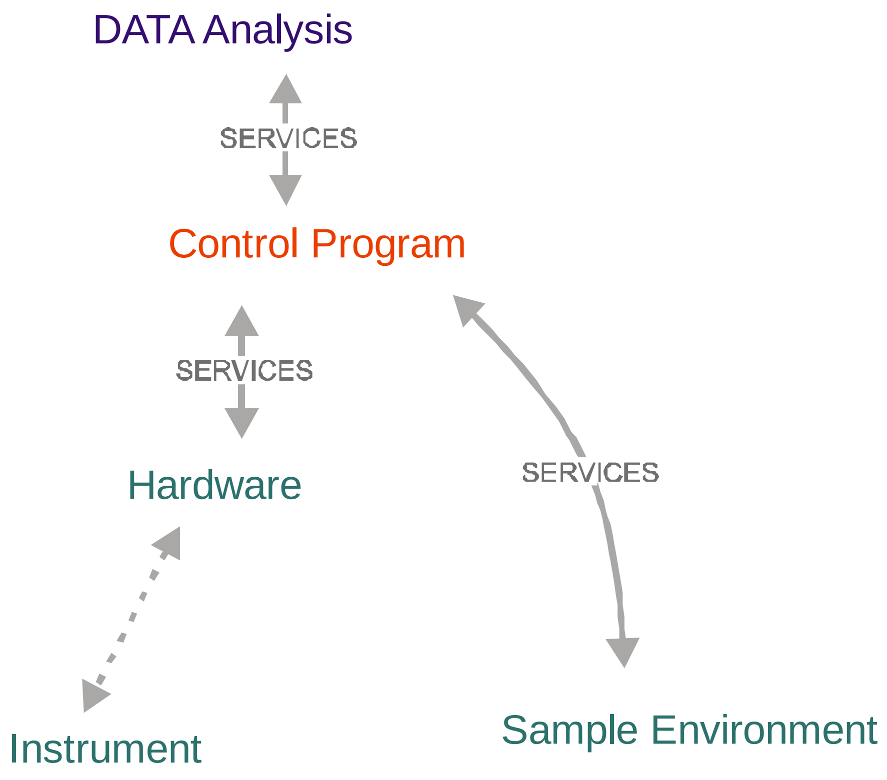


Figure 2: *Webservices Communication between nugget-like plug-in modules*

Action plan:

- Survey existing Nugget and potential needs, define technology for using Nuggets. This should include the guidelines/manual on the way how to proceed. Most platforms available commercially support the web-services (e.g., Labview).

- Pilot project can be the development of nuggets for sample environment control. In the same way that Nexus is a standard format one should look for a common agreement on web-service-like communication between the hardware control and the “intelligent” control server

General Recommendations:

- Physicists and Computer Scientists should work closely together and communicate
- More efficient beam time use by intelligent/dynamic experiment control, online data analysis (feedback from the control system)
- Communication of the facilities

The software of ANSTO, ILL and SNS is an open source and can be accessed by the internet for all interested end users.

5. SUMMARY OF INDIVIDUAL PRESENTATIONS

Presentations were made by each of the 6 experts describing their respective facilities, present developments related to data acquisition and analysis systems and future trends in this field both locally and world wide.

5.1. R.P. Schneider HZB, Germany

Promoting Reliability of Neutron Experiments by Harmonizing Interfaces, Formats and Routines

Recently the EU-project RESTAND within the framework of VAMAS TWA20 resulted successfully in a technical standard for the analysis of residual stresses by neutron diffraction. Based on that work we have already started a joint activity to form a network for development, validation, harmonization and standardization of techniques, procedures and tools used in residual stress and texture analysis, named STRAINET. The main outcome of this project shall be the enhancement of the repeatability and reliability as well as the convenience of residual stress experiments. Independently from the specific machine used, the standardization of procedures, data- and protocol formats as well as automation of calibration, measuring and data evaluation routines will result in an enhanced consistency of the results and more efficient instrument use. It is intended to facilitate joint research and development activities and finally to provide certified procedures.

For these types of especially dedicated instruments there is a common need to design and standardize an “expert-system”-like instrument control user-interface together with the complete experimental protocol, data formats (NEXUS) and data evaluation routines. As the core activity within STRAINET, this user-interface is intended to be jointly designed and developed, enabling comfortable instrument alignment, sample positioning, definition of scans, pre-evaluation of the current detector data, etc.

Additionally calibration and benchmarking samples have to be defined in order to validate and assess the instruments as well as the common developments. Benchmarking exercises assist not only in the enhancement of the reliability of experimental data, the validation of alignment and calibration routines, but also in analyzing strengths and weaknesses of individual facilities and to optimize experimental protocols.

This activity will strongly promote the International communication, the compilation and dissemination of knowledge on advanced experimental techniques and instrumentation. Finally we intend to come out with a common innovative tool for experiment planning, optimization, instrument control and data evaluation together with a definition of common formats and interfaces. The existence of a core activity of common interest will advance an efficient start of the network. An additional benefit of the proposed networking activity is the promotion of international co-operations in research, development and service for local industry. All developments within this project are freely available for all partners. All software developments are open source. The outcome of this cooperation will only be used for peaceful means. There are no additional restrictions in participating. All neutron facilities can benefit from the described developments and all of them are invited to contribute to the intended project.

Within this background at HZB a project, called “The Automatic Intelligent Experiment” has been started in close cooperation with Open University, Milton Keynes (UK). Here a strictly modular framework for the development of an “intelligent” user interface being currently developed that will enable the establishment of an “expert system” for residual stress analysis. This system can be either plugged on the various instrument control systems or adapted as stand-alone. This three year project is funded by HZB, FRM II and JRC.

substantial characteristics:
- intelligent instrument control and data evaluation tool
- open source software
- will be available via internet for free, no commercial packages included
- aspect orientated Java code, system independent
- strictly modular architecture, well defined interfaces (important for successful developments within an international network)

technical aims for stress and texture analysis
- automatic well documented instrument alignment and calibration
- special tools for user-friendly stress and texture experiments
- online data pre-evaluation
- CAD aided experiment planning, optimization and experiment control
- optical experiment surveillance, documentation
- artifact suppression by McStas Monte-Carlo experiment simulation
- NEXUS data format

To improve the efficiency of a residual stress diffractometer its components like detector, monochromator, sample-table, slit-system, collimators and the shielding can be improved in precision and quality. But another important characteristic of a diffractometer is the repeatability of sample positioning as well as the measured *d*-values even after a complete instrument re-alignment. Theoretically this does not increase the maximum possible precision in strain measurement due to the evaluation of relative peak positions only. But for the overall efficiency and reliability of the diffractometer it is a strong improvement to be able to measure repeatable absolute *d*-values within the usual error bars acceptable for residual stress analysis.

Using this framework a new instrument alignment system has been developed at HZB for highly accurate alignment and calibration of the HZB - residual stress diffractometers *E3, E7* as well as *Stress-Spec* at FRM II, recently. Using fully motorized slit-systems and a high resolution optical image processing system together with a set of standard-samples the instrument alignment and calibration is done fully remote-controlled by a computer. In the end a protocol displaying the alignment results gives information about all instrumental parameters together with their error bars.

5.2. R.A. Riedel, ORNL, USA

Achieving a common data ACQ architecture at the SNS and HFIR: challenges, opportunities and future plans

The SNS and HFIR facilities at ORNL are two neutron scattering facilities with significant operational and historical differences. In this paper we describe the unique features of each facility has they relate to data acquisition. Additionally we look at the effect of the history of data acquisition of each facility which also has a significant impact on the present status of the data acquisition. The areas in which both facilities can share data acquisition components are described.

The SNS is currently the highest power spallation source in the world. From the outset of planning for this time of flight neutron scattering facility the data acquisition group played a central role in the planning of control software and hardware for the neutron scattering instruments. One of the major challenges of the group was to improve the electronics design for neutron detector systems. A single well defined and detector interface is now in use for all operational and planned neutron scattering detector systems at the SNS. This commonality was achieved in spite of the wide differences in detector systems at the SNS. For example, 2D He gas detectors designed and built by BNL and acquired by SNS were modified by the DAQ group to meet the specifications required at SNS. These detectors are in use at the magnetism and liquid reflectometers. The same protocol because of its extensibility is also used for the large area instruments, ARCS and SEQUIOA which have approximately 140 He gas LPSD modules covering approximately 40 square meters. Scintillator based detectors used at SNAP, VULCAN and POWGEN were also designed using the same physical and logical interface. The conformity of all detectors at the SNS to the same standard proved to be an important reason that the DAS group is able to maintain and develop software for the operation of the instruments with a single common software package. The similarity of the interface allows one to design a set of abstraction classes providing an identical neutron scattering data format and control sequence independent of the instrument. The data format is known has event mode data which not only allows a common data format but will potentially allow a new class of scattering experiments to be run. The other aspect of data acquisition at the SNS is the control of ancillary equipment such has choppers motors, temperature controllers etc. Again a common well defined interface using a client server model was used. Although not an industry standard it uses a proprietary communications standard from National Instruments.

One key feature of the hardware control specification is that control of any hardware requires two graphical user interface (GUI) based applications. Both the server and client have GUIs. The use of a GUI in the server allows one to develop and use the server software has a stand alone application. This shortened both the software development and debugging time as well has providing an easy use hardware control application. The idea of "pluggablity" comes to play naturally with the system.

HFIR one of the worlds most powerful research reactors has a significantly different history of data acquisition. Until a year ago there was no central group for the development, design or maintenance of data acquisition or detector electronics. Also the detector electronics requirements are very different from the SNS. For example the most common detector is a single, single ended gas detector used on the three triple axis instruments. Other instruments use detectors designed by ORDELA and have a variety of physical and logical interfaces. The use of many interfaces makes software development more difficult. Also there is single abstraction layer within the software control architecture. This being said, one of the great successes in DAQ in the last four years was the development of the SPICE control software for the triple axis machines. This GUI based control software was developed with Labview software and has been well received by the user community. It was extended by other scientists for use at the two HFIR SANS instruments. Because no standard abstraction of the detectors exists, the software used at the triple axis and SANS instruments is not interchangeable. Other than the suite of detector electronics that must be supported at HFIR, the other major difference between the SNS and HFIR data acquisition systems is the lack of a server side GUI for hardware control.

It turns out that even with dissimilar systems there are important components of control that can be incorporated in both systems. The one item, surprisingly, that has little benefit in trying to make common is any drastic change in the overall system control or GUI structure. Because each facility has unique features, it is important to understand that at the level of user interaction, each facility requires a unique control GUI.

There are areas where significant commonality of software use can occur. Because of the client server model used at SNS it turns out to be relatively straight forward to add additional hardware drivers within the SPICE library to allow the use of both the SNS detector electronics and ancillary control hardware. This has already been done on two of the new instruments at HFIR and plans are being made to incorporate this functionality for all HFIR instruments so that a single SPICE package can be used at any scattering instrument at HFIR. The control protocol for ancillary hardware is currently under review by the DAS group for both SNS and HFIR. The goal is the transition from the current proprietary standard to a common industrial communication standard based on web services. This simple change would allow much of the control software developed at SNS to be used by the wider neutron community regardless of the particular control environment. In addition, various control packages developed at other institutions could be modified and used at the SNS.

5.3. M. Johnson, ILL, France

Current status and future directions for data analysis and related issues at ILL

The ILL operates about 40 instruments of which 25 are public and ~10 are operated by collaborating research groups. The instrument control service (SCI) lead by Mr Frederic Descamps provides hardware and software for data acquisition. The SCI group has in the last few years undertaken an important project to modernise the data acquisition software. The new program is called NoMad (replacing MAD, see http://www.ill.eu/science-technology/neutron-technology-at-ill/leading-edge-software-nomad/) and offers scientists an intuitive, user-friendly interface and many new possibilities, for example to easily incorporate non-ILL hardware, thereby facilitating new science.

On two new instruments, BRISP and IN5c, the long-standing ILL ascii data format is no longer tractable and NoMad produces NeXus files, which are becoming standard for neutron scattering (and X-ray synchrotron) data. The NeXus file content for IN5c will be compatible with NeXus data files produced on comparable machines at ISIS and SNS. Users of these facilities will therefore be able to use their preferred data analysis programs independently of the source of the data. This approach will be extended to other facilities and other types of data, enabled at ILL by the fact that the convertor for producing NeXus files from the NoMad, internal files exists.

Data analysis is a step further away from the instruments and data acquisition and a wide range of measurements and scientific fields have to be served by the analysis programs. Many programs exist: legacy codes, new codes and codes developed by instrument scientists and facility users. This wealth of routines and methods reflects the diversity of the scientific activity at a large scale facility. One role of the Computing for Science group (see http://www.ill.eu/computing-for-science/home/) is to support data analysis. By providing a common interface and infrastructure called LAMP, which is based on the scientific programming language IDL, re-use of existing routines is maximised and scientific input is reduced to short functions that are independent of reading raw data and plotting results.

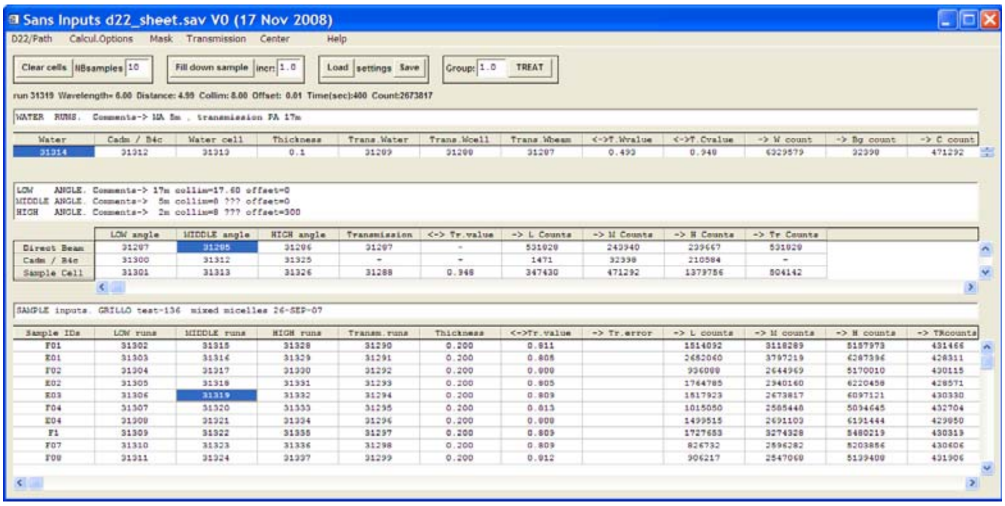


Figure: An example of a spreadsheet coupled to the data analysis program for treating small angle scattering data.

With increasing data rates, the emphasis in data analysis development is on new methods and workflow. A current example concerns data from small angle scattering (SANS) instruments, in which a large number of data sets have to be treated. Following an example from reflectometry, called COSMOS, we are now investigating the use of a spreadsheet in LAMP (SANS sheet, see below) to pass the information to the core data analysis code in one-go. The advantage of this approach is that spreadsheets are typically employed by users to record the experiment protocol and they give a clear overview of the whole experiment.

5.4. J. Li, CIAE, China

The New Developing Control and Data Acquisition System for Residual Stress Instrument in CIAE

China's first research reactor, Heavy Water Research Reactor(HWRR), was built in 1958 in CIAE, the fuel enrichment was 2 % ^{235}U at that time, and the Power is 7MW (maximum power 10MW). Maximum thermal neutron flux in the core is $1.2x10^{14}n/cm^2/s$. HWRR was upgraded in 1979-1980 to 10 MW, maximum thermal neutron flux in the core is $2.8x10^{14}$ $n/cm^2/s$. Collaboration with the neutron group from Institute of Physics, CAS, TAS, FCD and SANS had been introduced into CIAE in 1980s. The reactor had been shut down in 2007.

At present, a 60 MW tank-in-pool inverse neutron trap-type research reactor, China Advanced Research Reactor (CARR), is being built at China Institute of Atomic Energy (CIAE) in Beijing. CARR is indeed a multiple purposes research reactor, and neutron scattering (NS) is a major research program opening to users from universities, industry and government labs. The key parameters of CARR are listed as follows: the power is 60 MW, max undisturbed thermal neutron flux is $8x10^{14}$ $n/cm^2/s$ (at heavy-water reflector), U^{235} enrichment is 19.75 %, 7 of 9 horizontal beam tubes will be used for NS.

The Phase I instruments constructed in NSL of CIAE are listed below:

30-m SANS Instrument, horizontal-sample-geometry Reflectometer, Residual Stress Diffractometer, Triple-axis Spectrometer, Four-circle Single-crystal Diffractometer, High-resolution Powder Diffractometer, High-Intensity Powder Diffractometer, TOF Spectrometer and neutron radiography instruments.

These instruments have got different software, so we have strong demand to learn and adopt a standard data acquisition and analysis systems. Fortunately now we can refer to the LAMP and Gumtree systems which are free to download from the website. Harmonization and standardization of data acquisition and analysis systems is desirable and practically feasible.

The Residual Stress Diffractometer is one of the first facilities to be built at CARR to meet the demand of industrial application of non-destructive stress measurement. The software of motion control and data acquisition system is being developed in-house using Labview. Following the recommendations of this consultancy meeting, the data format of this instrument will use NeXus data format. In the future we will improve this system with a standardization of data acquisition, interfaces and data analysis procedures.

5.5. M. Shaat, RR Centre, Egypt

Application of Data Acquisition System for Research Reactors and Experiments

Egypt presently owns two research reactors:

1. The first one is called ETRR-1, was built by the former USSR, and was commissioned in 1960. The purpose of that reactor is R&D, isotope production, training and applying nuclear physics experiments. The reactor operates at 2MW power, is a tank type, using EK-10 fuel with 10 % enrichment, and the reactor equipped with nine vertical irradiation positions and nine horizontal beam tubes and thermal column. The reactor provides a thermal neutron flux of the order of 1.5E13 $n/(cm^2\,s)$, and is using light water as coolant and moderator.

2. The second reactor is called ETRR-2 and was built in cooperation with Argetina. The reactor was commissioned in 1997, with the main purpose of production of new radio-isotopes, which require high flux and long irradiation time. Presently the reactor operates at 22 MW thermal power. It is open pool type reactor using plate fuel elements with 19.75 % enrichment. In addition to isotope production, the ETRR-2 reactor has facilities for NAA, Neutron radiography, and Neutron silicon doping. There is an ongoing IAEA TC project for development the beam tube experiments and to install a SANS-type experiments.

For the control of the ETRR-1 reactor a real – time computerized data acquisition was installed in 1995, which is based on the advanced technology of programmable controller (PLC). Its software depends on the LABTECH control and VISION programs for data logging and real time representation. The DAS is used for:

- Data logging and analysis for the reactor performance, especially after transient events
- Records and log book
- Archives and data storage
- Data provision for the reactor users and to support the operators during abnormal reactor operation.

This DAS can display the information in the form of graphics, tables and schematics. The ETRR-2 Reactor has experimental beam line tubes as:

-Neutron time of flight (TOF)
- Neutron diffraction (single crystal)
- Computerized neutron tomography (CNT)
- Neutron scattering
- Powder diffractometer.

The neutron beam line facilities for ETRR-2 reactor like neutron radiography, NAA and neutron transmutation doping have their dedicated data acquisition and analysis software. For future development of our facilities, e.g. digitalization of the existing neutron radiography facility or for the new beam line applications, we intend using the advanced and standardized data formats and software for better data acquisition and analysis.

5.6. O. Kirstein, ANSTO, Australia

Community based software solutions for data acquisition for neutron scattering experiments at ANSTO

The Neutron Beam Instrument Project (NBIP) which was a sub-project of the Replacement Research Reactor Project at the Australian Nuclear Science Organization ANSTO finished recently in May 2008. Part of this project were eight neutron scattering instruments and an IT/computing project which was designed to provide not only motion/instrument control but also data acquisition and data analysis. In hindsight there are a few lessons learnt that could benefit new projects with a similar scope – in particular at new research reactors.

Right from the beginning a close relation with the user community of the neutron scattering instrumentation was established by organizing workshops during which the community were asked to articulate their wishes. Constant interaction with the user community (including the instrument scientist responsible for the respective instrument) and feedback turned out to be successful. For ANSTO / NBIP standardization not only in terms of hardware but also in terms of e.g. graphical user interfaces turned out to be successful. Whereas hardware standardization is an effective way to overcome hardware failures in a user facility standardization of graphical user interfaces amongst at least classes of instruments (e.g. powder diffractometers) guides and helps users to control the instrument and carry out their experiments as efficiently as possible.

The use of up-to-date client server architecture, frameworks, scripting and development environments (e.g. Java, Eclipse, Python) that are supported by industry and a broader community than the neutron scattering community only minimizes development and maintenance and gives the opportunity for the local IT department to focus on special applications typical for local neutron scattering instrumentation, which often requires specialized data treatment. Using Open Source project such as Gumtree, OpenInspire, Lamp also minimizes local effort allowing the IT group to focus specialized site-wide applications. Establishing collaborations is another beneficial way to share the workload and gain experience at the same time (e.g. ANSTO collaboration with Paul-Scherrer-Insitut PSI, Switzerland with regards to instrument control SICS and ESRF, France with regards to GUI / analysis software - Gumtree). Standardized file formats such as NeXus simplify data analysis and minimizes the effort to adopt specialized programs to laboratory specific data formats. Of course, introducing frameworks, development environments or file formats is easier if the infrastructure is being built from scratch.

In summary,

- Application of best practice in systems engineering and project management
- System Modelling
- Minimisation of code development
- Use industry standard components
- Use frameworks e.g. Eclipse
- Benefit from already available code/applications/plug-ins via collaboration

will be an effective way to provide a framework for an IT group in particular at new facilities that wants to benefit from the wealth of experience that is already available at other well established facilities such as ILL, SNS-HFAR, ANSTO.

6. DISCUSSIONS AND RECOMMENDATIONS

The meeting participants agreed that a better coordination and organization is urgently needed as long as data acquisition and analysis systems for neutron beams are concerned, and therefore the assistance from the Agency in terms of networking within this topic was recommended.

Nexus is becoming a standard data format for neutron scattering and x-ray experiments, what ensures/facilitates the exchange of the data for multiple users, permits the decoupling of the data source and the various analysis methods.
R1: the actions should be taken to encourage and assist new neutron beam facilities/applications in the use of data format based on NeXus. This could be realized in cooperation with the IAEA within the pilot project related to the residual stress measurements (STRAINET).

Modular development of acquisition and analysis software facilitates standardization and ensures flexibility and reuse across facilities, that could guarantee the facility/user independence
R2: the assistance is needed to facilitate and support fellowship program for international exchange and training (e.g. researchers from emerging new facilities will be hosted by the established facilities for the training both in hardware and software for neutron beam applications).
Potential fellowship projects might be: 1) Review of current best practices driven by new developments at emerging and established facilities used to lever common trends and evolve standards related to modularity. The Agency should try to encourage new projects to work along and implement the defined standards, 2) Realization of well-defined modules using standard communication interfaces as web services (e.g. local sample environment: high-temperature furnace on the powder diffraction instrument) in order to facilitate standardization at the international level.

Centralized information would strongly facilitate the implementation of the above recommendations.
R3: the assistance is recommended in: a) establishment of a data base on data acquisition and analysis for neutron beam applications hosted and managed at the IAEA, b) transfer of information about related topical meetings (NIAC, NOBUGS) on a dedicated web-page and support the participation from developing member states.

New neutron beam facilities should start from the best available practices as long as data acquisition and analysis are concerned, and if possible, immediately from the standard ones.
R4: the actions should be taken to encourage and support established topical data acquisition and analysis conferences/workshops to be organized at the facilities in the developing countries with advanced new neutron beam projects (e.g. China, South Africa, etc.).

The promotion of Neutrons for Science through the virtual “Neutron Flight Simulator” was discussed and endorsed.
R5: the recommendation is made to participate in promoting the use of neutron beam experiments through virtual experiments, assist in creation and distribution of a toolkit for the production of numerical data using McStas description of instruments at existing facilities (e.g. in this way training for data analysis based on numerical data could be achieved/promoted/explained before the real experiment takes place).

7. LIST OF PARTICIPANTS

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8. AGENDA

Wednesday, 10 December 2008

08:30 - 09:30	Arrival/Registration: Gate 1
09:30 - 10:00	**Welcome** Opening remarks *Mr G. Mank* (Head, NAPC / Physics Section) *Mr D. Ridikas* (RR Officer, NAPC / Physics Section) Background and Goals of the Meeting Nomination of Chairperson, Reporter(s) and Facilitator(s)
10:00 - 11:00	**Presentations (50 min + 10 min discussion)** *Mr R.P. Schneider* (HMI, Germany)

"Promoting Reliability of Neutron Experiments by Harmonizing Interfaces, Formats and Routines"

11:00 - 11:30	Coffee break
11:30 - 12:30	**Presentations** (continued) *Mr R.A. Riedel* (ORNL, USA)

"Achieving a common data ACQ architecture at the SNS and HFIR: challenges, opportunities and future plans"

12:30 - 13:30	Lunch break
13:30 - 14:30	**Presentations** (continued) *Mr M. Johnson* (ILL, France)

"Current status and future directions for data analysis and related issues at ILL"

14:30 - 15:30	**Presentations** (continued) *Mr J. Li (CIAE, China)*

"The New Developing Control and Data Acquisition System for Residual Stress Instrument in CIAE"

15:30 - 16:00	Coffee break
16:00 - 17:00	**Presentations** (continued) *Mr M. Shaat (RR Centre, Egypt)*

"Application of Data Acquisition System for Research Reactors and Experiments"

17:00 - 18:00	**Presentations** (continued) *Mr O. Kirstein (ANSTO, Australia)*

"Community based software solutions for data acquisition for neutron scattering experiments at ANSTO"

18:00 - 18:30	**Discussion and Summary of all contributions**

Thursday, 11 December 2008

09:00 - 11:00 **Discussion (1) on**

- Breakthroughs in R&D on data acquisition and analysis systems in emerging neutron beam applications as Quasi-Laue Diffraction, Ultra-SANS, 3D Neutron Tomography, etc. (e.g. country/region reports, publications, conference presentations, etc.)

11:00 - 11:30 Coffee break

11:30 - 12:30 **Summary of Discussion (1)**

12:30 - 13:30 Lunch break

13:30 - 15:30 **Discussion (2) on**

- Needs on unification and standardization of data acquisition and analysis for neutron beam line experiments (e.g. residual stress measurements, neutron radiography, etc.); identification of neutron beam applications, where RR user networks could be initiated in relation with harmonization and standardization of data acquisition and analysis

15:30 - 16:00 Coffee break

16:00 - 18:00 **Continuation and summary of Discussion (2)**

19:00 - **Hospitality**

Friday, 12 December 2008

09:00 - 11:00 **Discussion (3) on**

- Role RRs can play in development and testing of dedicated data acquisition and analysis systems to be used in new generation spallation neutron sources; identification of possible synergies

11:00 - 11:30 Coffee break

11:30 - 12:30 **Summary of Discussion (3)**

12:30 - 13:30 Lunch break

13:30 - 15:30 **Preparation of the summary report and recommendations**

15:30 - 16:00 Coffee break

16:00 - 17:00 **Final conclusions, follow up and meeting closure**