



canSAS V

Workshop Report

The Fifth canSAS meeting was held on October 29th to 31st on the NIST campus in Gaithersburg, Maryland, hosted by the NCNR SANS group. The aim of the international organizing committee was to keep the group to a reasonable size of motivated people to have frank and open discussion of issues and work on solutions that would be outcomes of the meeting. The format included oral presentations, posters, and software demos as well as plenty of discussion time from moderated discussions, to open discussions, to various informal discussion opportunities. The workshop was successful at stimulating significant levels of interactions and lively discussions.

The following six points are the result of that meeting and the outcomes agreed to at the final session on Wednesday morning. Most of them consist of the formation of working groups to keep the momentum going on issues that showed promise at the meeting:


I. Facility Representatives Discussion Group

There was agreement to form some kind of Facilities Representatives Discussion Group (FRDG) that should meet two to four times a year by teleconference. Preference for videoconferencing when possible was expressed. Also a mailing list might be an appropriate means of arranging the meetings, circulating agendas, and extending discussions.

It was envisaged that this group should not be seen as those who will carry out all the work or have all the answers. Rather they will be a contact group who will bring in their local experts to deal with issues as needed. Briefly noted were the conflicting requirements of keeping the group small enough to be manageable while being as inclusive as possible. Clearly details still need to be worked out and Paul Butler agreed to spearhead this effort.

The following issues were brought up at the workshop but were not assigned immediate actions and need further discussion. These could be suitable subjects for this forum:

1. Co-refinement issues
2. Preservation of data issues
3. Auto-capturing and storing of meta data
4. Qz issues (both in terms of data sampling and resolution)
5. Resolution issues and how to educate users to their relevance
6. Naming convention for reduced data (also to be explored by format group)
7. Higher order reduced data sets (1, 2, 3, 4... etc)
8. Libraries and binary repositories of code – should use portal. Standard should accommodate both validated and “seat of pants” code. Linux model was suggested as an example
9. Sharing information on current individual facility initiatives and discussion of possible collaborative initiatives



10. Next Generation software support: How do we design and deploy our software to enable the science

- a. Design to various level of users
- b. Real time fitting @ beamline
- c. Experiment planning (include simulations)
- d. New software tools (SASSIE, LORES, “microscope”)

The following people expressed interest in participating in this process:

- Peter Boesecke (ESRF)
- Paul Butler (NIST)
- Daniel Clemens (Germany)
- Charles Dewhurst (ILL)
- Elliott Gilbert (ANSTO)
- Rex Hjelm (LANSCE)
- Pete Jemian (APS)
- Steve King (ISIS)
- Ken Littrell (ORNL)
- Adrian Rennie (Users)
- Nick Terrill (Diamond)

Timetable:

- First meeting to be organized in first quarter of 2008


II. 1D Data Formats

A working group on 1D formats was formed. After some heated debate over the proposal brought forward by Steve King and Ron Ghosh, an XML 1D format, with 4 default columns defined and others left to individual facility discretion, was agreed on in principle. Many details were worked out at the meeting but a working group was formed to finalize and circulate a final proposal by the end of 2007. It was suggested that this group also consider the feasibility of file naming convention but that failure to make progress in that area should not slow the process of adoption of the file format itself. Also noted was the similarity to reflectometry data and the fact that at some point it might be appropriate to contact that group.

Marc Malfois noted that the IUCr SAS CIF format had just been ratified while Pete Jemian indicated that the SAS NeXus format was “very close” and would probably be ratified by the next NIAC meeting expected in the second half of 2008. The working group was encouraged to keep naming conventions compatible with the NeXus standard. Pete Jemian being involved with both groups would help ensure this.

The working group consists of:

- Andrew Jackson (NIST)
- Pete Jemian (APS)
- Steve King (ISIS)
- Ken Littrell (ORNL)
- Andy Nelson (ANSTO)
- Ron Ghosh (ILL) *
- Jan Ilavsky (APS) *



* Jan and Ron stated that they wanted to be “in the loop” but not necessarily be directly involved in the decision making.

Timetable:

- Final proposal for minimal file definition circulating by end of 2007.
- Names of first facilities implementing standard available by first meeting of FRDG.
- 1st draft of proposal for 2D reduced format by SAS 2009

III. IGOR Developers

An IGOR working group was formed to address issues common to all the IGOR SAS developers. Whilst it was felt that the IGOR SAS developer community was basically present at the workshop, the IUCr sa_scat list might be used to find other interested parties.

The purposes of the group were seen to be:

1. Developing common documented practices, particularly as regards procedure naming conventions which can lead to conflicts between IGOR packages.
2. Promoting a web page for SAS IGOR code sharing (should link from portal)
3. Developing a common library of documented reusable code
4. Developing common 1D loaders for data

The working group consists of:

- Jan Ilavsky (APS)
- Andrew Jackson (NIST)
- Steve Kline (NIST)
- Ken Littrell (ORNL)
- Andy Nelson (ANSTO) (chair)

Timetable:


- Report on agenda and timetable for agenda by first FRDG meeting
- Have most in place by Sydney nobugs meeting (fall 2008)

IV. Global SAS Web Portal

The idea of a global SAS portal was presented by Steve King and was strongly supported. A central web presence that is the first place that comes to mind whenever a SAS question comes up is overdue. The demise of CCP13 funding may serve as the catalyst for this. It will however require resources to actively maintain the relevance of the site. Web technologies however mean that all need not reside on a single sever nor is only one person required to do all the work. NIST, the eScience group at STFC (L Lerusse), and DANSE SANS group offered support.

A working group was formed consisting of

- Andrew Jackson (NIST)
- Steve King (ISIS)
- Jonathan Rawle (Diamond & ISIS)



Many issues were raised that will need to be addressed to make this endeavor successful:

1. Facilities must be strongly encouraged to point to the portal and the portal must link to all facilities
2. The canSAS pages should be move to the site as a new home will be required with Ron Ghosh's retirement.
3. small-angles.ac.uk (ISIS/King has content) and smallangles.net (Jackson has canSAS-V website and mailing lists) should arrange to merge in some fashion
4. The World SANS directory needs to be kept more current (will require somebody who can pro-actively update it on a fairly frequent basis, particularly with the wave of new SANS instruments coming on line worldwide). The ILL would like to continue hosting it, but with the retirement of Roland May, Peter Timmins will work to identify a new person at ILL for this task.
5. A world wide SAXS directory would also be a good idea – Pete Jemian will look into what resources are available to build it.
6. The hosting of, or linking to, subversion repositories was seen as a means to encourage and support collaborative and/or co-operative projects (Source Forge for SAS). Examples from the meeting include: CCP13, MOTOFIT, NIST IGOR, DANSE. J Curtis (SASSIE) is interested in discussing this idea also.
7. The portal should provide a place for, or pointers to, other (and all) SAS code repositories.
8. The IUCR sa_scatter mailing list should be clearly advertised on, and accessible from, this page. The site should also provide other, more specialized, mailing lists (lists for the working groups was an initial example)

Timetable:

- Mailing lists up by end of November (Done November 6th)
- Merging of small-angles and smallangles by April 2008
- Have most of the rest ready by nobugs in Sydney in fall of 2008


V. Standardization

A Standardization and QA working group was formed, initially including:

- John Barker (NIST)
- Peter Boeseke (ESRF Contact)
- Stephen Henderson (UMD)
- Rex Hjelm (LANSCE)
- Jan Ilavsky (APS)
- Peter Lindner (ILL)
- Marc Malfois (Diamond)
- Adrian Rennie (Uppsala University - chair)

There were three suggested modi operandi for the group and a mix of all rather than only one method was promoted.

1. Run agreed standards regularly. Possible standards suggested at meeting were:
 - a. Glassy Carbon (Jan Ilavsky has standard)
 - b. Ag Behenate – issues mentioned but currently seems reasonable

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- c. ORNL (Wignall) standards
 - d. Holographic grating (Dewhurst)
 - e. Polystyrene spheres (what size?)
 - f. C60 in CS (see Henderson work?)
2. Periodically run some “real” samples as round robin to test “real world” responses of instrumentation (high intensity, low intensity, steep slopes, flat scattering, peaks, Rg etc etc)
 3. Facility exchanges where one person with a sample travels to 2 or more facilities to run the experiments. Henderson points out benefit of this in terms of actually working things out while others point to the benefits of personnel interchange.

The purposes of the working group were seen to be:

1. To define appropriate standard protocols and processes for best ensuring standardization.
2. To identify initial facilities for involvement (3-5 each of neutron and X-ray)
3. To verify management support for the process
4. To identify protocols, what to report and how, for each type of test – Reports should be available on global portal web pages
5. To eventually explore funding options (NMI3 was suggested as a possible source for the European side)

It was envisaged that the results of the standardization would lead to a “quality mark” from the group for facilities that are involved. The idea being that users could be confident that results they obtain from those facilities would be comparable.

Timetable:

- Develop a plan for the path forward with timetables by first meeting of FRDG.

VI. Workshop Themes

There were a number of general themes of the meeting that were not action items themselves but capture the overall “sense of the workshop”

1. The participants strongly support the idea of open development of SAS software. This is both for reasons of collaboration and for openness of the scientific process through examination by others of details of methods used.
2. The participants strongly encourage facilities to publish the definition of all formats they use such that a newcomer can immediately comprehend said formats.
3. The participants also encourage facilities to provide the means to read their data. This could be a library, code examples, or converters to the to-be-agreed XML format.
4. The participants strongly encourage SAS software developers to publish a clear definition of the inputs their code expects as well as the definition of any outputs, in particular details of the output parameters, from their code. This aims to more easily allow meta-analysis of the scattering data by aggregation of fitting results.

Workshop Attendees



Back Row (L-R): Ron Ghosh, Peter Timmins, Adrian Rennie, David Mildner, Lauent Lerusse, Marc Malfois, Ken Littrell, Steve King, Jan Ilavsky, Stephen Henderson, Jonathan Rawle,

Middle Row (L-R): Andy Nelson, Paul Kienzle, Andrew Jackson, Rex Hjelm, Peter Boesecke, Boualem Hammouda, Helmut Kaiser

Front Row (L-R): Pete Jemian, Steve Miller, Paul Butler, Mathieu Doucet, Lionel Porcar, Charles Dewhurst, Steve Kline, John Barker, Daniel Clemens

Not present for photograph: Michael Agamalian, Joeseeph Curtis, Susan Krueger, Mark Laver, Mike Martin, Michihniro Nagao, Cameron Neylon, Xiangyun Qiu, Bob Shirley, Piotr Zolnierczuk