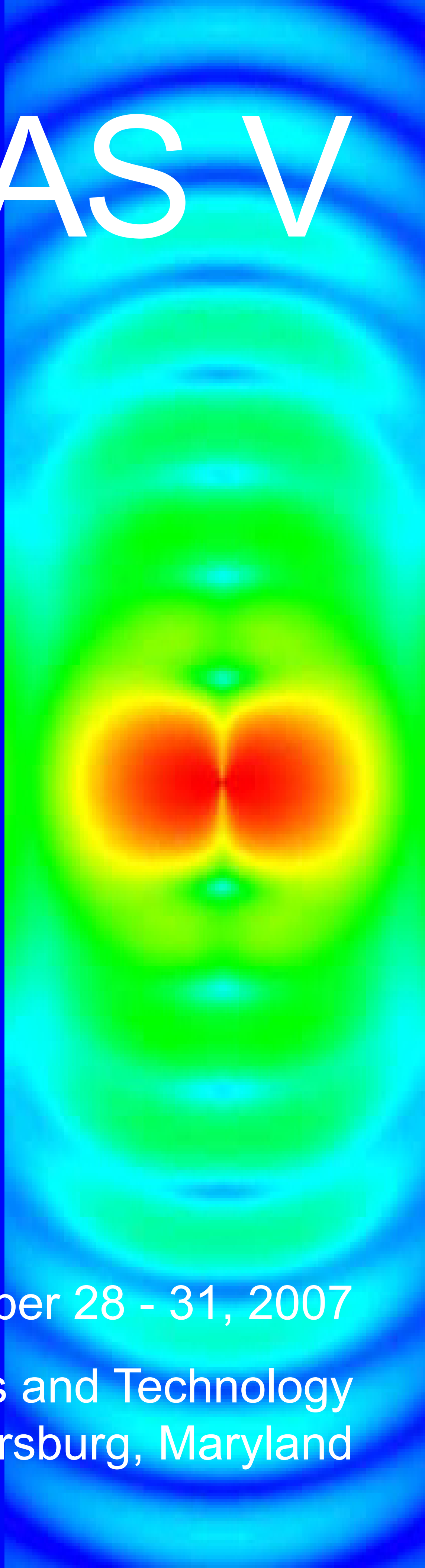
canSAS V



October 28 - 31, 2007

National Institute of Standards and Technology
Gaithersburg, Maryland

Meeting Sponsored By

Welcome!

This is a “packet” of information about the workshop. If you lose everything else feel free to call us for help/directions.

Some useful numbers:

Paul Butler’s cell phone:		865 387-2047
Andrew Jackson cell phone:		240 361-8622
Conference services:	Angela Ellis	301 975-3881
	Mary-Lou Norris	301 975-2002

Bus pickup a the hotel will be 8:30AM (for a 9AM start). It is assumed that those of you staying at the hotel will have had breakfast there and only coffee, tea and juice will be available on arrival in morning. Morning break will have snacks and drinks.

We hope you will already have thought about what you think are important issues you want discussed as well as things you might want to see come out of the workshop. For those of you speaking “officially” please keep your talks to 20min or less as we want to maximise debate. There will be chance during the discussions for short (sub 5 minute) “presentations” so if you have a couple of slides that you think might be relevant to the discussion please have them ready!

As you can see there are plenty of opportunities for discussion and we plan to let the schedule be flexible enough to adjust to needs identified by the delegates (without degrading into chaos). Brief few minute presentations will be possible during discussions so come ready to participate.

We are looking forward to a lively and productive workshop.

Paul Butler and Andrew Jackson

on behalf of the Organizing Committee:

Steve King (ISIS)
Adrian Rennie (Uppsala University)
Nick Terrill (Diamond Light Source)
Satoshi Koizumi (JAEA)
Elliot Gilbert (ANSTO)
Peter Jemian (APS)

Workshop goals and vision

Given that facilities will always be a slave to NIHS (not invented here syndrome) what can be done to minimize the impact on border blind Bedouins?

In the past such meetings as this, nobugs, and others have focused on the vain hope that time and volume of meetings would eventually be sufficient to force significant changes. This has had only marginal success by any measure and been an abject failure by the cynics' telling. canSAS was partly a hope that the nomads themselves would create solutions, but Bedouins tend to have a very narrow focus on "me" and "today." What is needed is a new more pragmatic approach to enhancing the nomadic quality of life.

The approach of the canSAS V workshop therefore is to focus on fostering and encouraging discussions at many levels yet have those discussions guided enough for some tangible results to be possible.

Series of short talks on needs, state of the art, and future directions in particular topical areas are followed by an open or moderated discussion as appropriate, with the ability of participants to get up and give ~3 minute mini presentations to make a point. Generous time for breaks and poster sessions/demonstrations provide an opportunity for focused yet less structured discussions, while the accommodation venue was chosen to allow less focused and free flowing interactions.

Finally, the closeout session of the workshop is designed to tie as much of the results as possible together and produce a set of outcomes where appropriate. The idea is to steer away from the one size fits all solutions to simpler "lowest common denominator" solutions. Throughout, the hope is to remain flexible enough for the schedule to shift dynamically to fit the needs of the participants.

The topics were initially chosen by asking what the main issues facing the nomad are. This process generated to the following list:

- Making sure the data is correct no matter what facility it come from (how do we know?)
- Figuring out how to correct for the resolution for a given facility
- Figuring out how to extract the information from the data
- Simultaneously fitting of data from various facilities (neutron and x-ray)
- Keeping up with the latest developments in software so as to be able to focus on the interesting science instead of wasting time re-inventing the wheel.

Thinking about the list above lead to the following broad categories of issues that could enhance that gypsy experience and became the original topical areas:

- Data formats
  - 1D, 2D, and metadata
  - Resolution
    - What is "correct" method for dealing with resolution
    - Different needs for SAXS, SANS, and USAS
    - What should be required so that any method will work (i.e. to make everybody happy)
  - Possible outcomes:
    - Common interchange format for SAS
    - Software library routines conforming to some standard
    - Other determined as the workshop develops

- Software tools
  - What is available and where are things headed (new models, new methods, speed improve ments, distributed/grid computing, etc)
  - What are people doing but not sharing
  - How can we share better – possible outcomes
    - Vibrant SAS portal/repository – what would be the requirements?
    - Collaborative development a la open source – what would be requirements?
    - Common validated C library building blocks. What would be the requirements
    - Other ideas developed by the workshop.

- QA/ standardization
  - Nomads always carry their own "gold standard" sample
  - What are the experiences in this area?
  - What can facilities be expected to do to minimize problems – suggestion:
    - Yearly round robin with variety of constantly changing samples
      - Allow facilities to detect problems early
      - Give more confidence to nomads
      - Enhance inter facility interactions which should lead to many unanticipated benefits and novel developments.
  - Other ideas developed by the workshop.

Finally, you should keep in mind that this write-up is meant to generate discussion and ideas and not meant to dictate the final agenda which, as mentioned at the start, should be guided by **you** and the unknown path the discussions will lead us.

Schedule

Sunday October 28th 2007	
19:00 onwards	**Informal gathering** Uncle Julio's Rio Grande Cafe Washingtonian Center
Monday October 29th 2007	
09:00 - 09:15	**Workshop Overview** Welcome and workshop objectives Speaker: Pat Gallagher and Paul Butler
09:15 - 10:30	**Software - Advanced Data Analysis (building a better camel)** Presentations on trends, developments and current state of the art in data analysis software. Speakers: C Dewhurst, J Ilavsky, J Curtis Open Discussion
10:30 - 11:00	**Break**
11:00 - 12:15	**Software - Advanced Data Analysis (building a better camel)** Presentations on trends, developments and current state of the art in data analysis software. Speakers: L Lerusse, M Malfois, M Agamalian, Open Discussion
12:15 - 13:30	**Lunch**
13:30 - 14:45	**Software - Advanced Data Analysis (building a better camel)** Presentations on trends, developments and current state of the art in data analysis software. Speakers: M. Doucet, P Kienzle, A Nelson Moderated Discussion
14:45 - 15:15	**Break**
15:15 - 16:30	**Software - Collaboration and Development** Speakers: A Jackson, S King, S Miller Moderated Discussion
16:30 - 18:30	**Software Demos and Poster Session**
18:30	**Bus to Hotel**
Evening	**Open**

Tuesday October 30th 2007	
09:00 - 10:30	**Data Formats - Resolution** Presentations of resolution issues: how to correct and how to carry the information in the data Speakers: J Ilavsky, B Hammouda, K Littrell, D Mildner Open Discussion
10:30 - 11:00	**Break**
11:00 - 12:45	**Data Formats - Requirements** Presentations on data format issues Speakers: S King, P Boesecke, C Neylon Moderated Discussion
12:45 - 14:00	**Lunch**
13:30 - 15:15	**Standardization** Presentations of issues of data comparison between facilities Speakers: R Hjelm, S Henderson Moderated Discussion
15:15 - 16:30	**NCNR Tour** Tour will be in small groups during this session. Alternatives will be available for those not interested in the tour.
16:30 - 18:30	**Software Demos and Poster Session**
18:30	**Bus to Hotel**
Evening	**Group Dinner** At Macaroni Grill, Washingtonian Center

Wednesday October 31st 2007	
09:00 - 11:00	**Workshop Wrap-Up** General discussion and loose ends of issues from previous 2 days Moderated Discussion
11:00 - 11:30	**Break**
11:30 - 12:00	**Workshop Close-Out** Conclusions and Outcomes Leader: Paul Butler
12:00 - 13:00	**Lunch**

To NIST

Driving Directions from Washington Dulles International Airport (IAD)

Follow the Dulles Access Road to Bethesda/Baltimore entrance ramp to 495
Take 495 (left lane exit) to 270 North
Take 270 Local North toward Montrose Road
Take Exit #10 toward Clopper Road (MD 117) and Quince Orchard Rd (MD 124)
At the first light turn right onto Clopper Road.
At next stop light (Bureau Dr.) turn left

Driving Directions from Baltimore Washington International Airport (BWI)

Take 195 West
Take 95 South Exit #4B toward Washington
Take 495 West Exit #27-25 toward College Park/Silver Spring
Take 270 North Exit #35 toward Frederick
Take 270 Local North toward Montrose Road
Take Exit #10 toward Clopper Road (MD 117) and Quince Orchard Rd (MD 124)
At the first light turn right onto Clopper Road.
At next stop light (Bureau Dr.) turn left

Driving Directions from Ronald Reagan Washington National Airport

Exit National Airport heading north on the George Washington (GW) Parkway toward Maryland
Take the GW Parkway to 495 North toward Maryland
Take 495 (left lane exit) to 270 North
Take 270 Local North toward Montrose Road
Take Exit #10 toward Clopper Road (MD 117) and Quince Orchard Rd (MD 124)
At the first light turn right onto Clopper Road
At next stop light (Bureau Dr.) turn left

To Hotel

Hotel Address for Cabs or Limos
9721 Washingtonian Blvd.
Gaithersburg, Maryland 20878 USA
Phone: 1-301-590-3003

Driving Directions from Washington Dulles International Airport (IAD)

Follow the Dulles Access Road to Bethesda/Baltimore entrance ramp to 495
Take 495 (left lane exit) to 270 North
Take Exit #8 toward Shady Grove Road West.
Turn left on Shady Grove Road.
Shortly thereafter turn right onto Research Boulevard.
At Omega Drive turn right.
At Washingtonian Boulevard (traffic lights) turn right.
The Residence Inn is on the right after you pass the Springhill Suites Hotel.

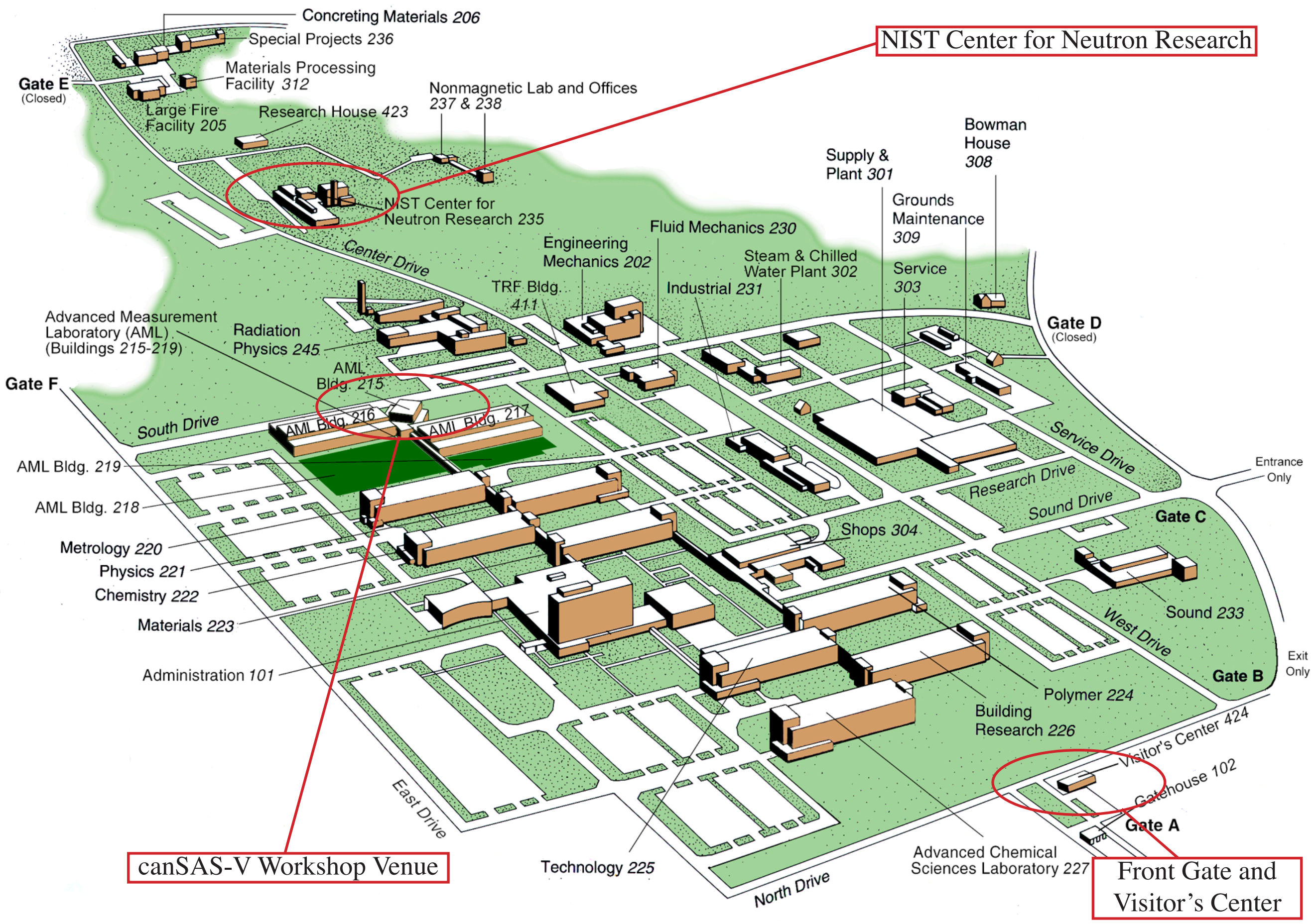
Driving Directions from Baltimore Washington International Airport (BWI)

Take 195 West
Take 95 South Exit #4B toward Washington
Take 495 West Exit #27-25 toward College Park/Silver Spring
Take 270 North Exit #35 toward Frederick
Take Exit #8 toward Shady Grove Road West.
Turn left on Shady Grove Road.
Shortly thereafter turn right onto Research Boulevard.
At Omega Drive turn right.
At Washingtonian Boulevard (traffic lights) turn right.
The Residence Inn is on the right after you pass the Springhill Suites Hotel.

Driving Directions from Ronald Reagan Washington National Airport

Exit National Airport heading north on the George Washington (GW) Parkway toward Maryland
Take the GW Parkway to 495 North toward Maryland
Take 495 (left lane exit) to 270 North
Take Exit #8 toward Shady Grove Road West.
Turn left on Shady Grove Road.
Shortly thereafter turn right onto Research Boulevard.
At Omega Drive turn right.
At Washingtonian Boulevard (traffic lights) turn right.
The Residence Inn is on the right after you pass the Springhill Suites Hotel.

NIST Campus Map



The workshop is being held in the conference room of the Advanced Measurement Laboratory (AML), Building 215 on the NIST Gaithersburg Campus.

If you are arriving by bus from the hotel, you will be greeted at the Visitor's Center by Conference Services staff who will provide you with your badge.

If you are arriving by car you will need to go to the Visitor's Center to obtain your badge. To get to the Visitor's Center keep right as you drive up to the main gate and then bear right into the car park, following the traffic cones.

The Washingtonian/Rio Center has a variety of restaurants, cafes and shops and is an easy 5 to 10 minute walk from the Residence Inn.

To get there, leave the hotel and turn right down Washingtonian Boulevard. When you reach the Marriott Courtyard hotel (a tower building) walk down to the lake and along the boardwalk

Tuscan

Includes appetizer, salad, entrée, dessert and non-alcoholic beverage.

Salad

Choice of House Caesar or Garden with sweet Italian vinaigrette dressing.

Antipasti

Calamari Fritti Crispy, tender calamari served with pizzaiola and basil pesto aïoli.

Shrimp & Artichoke Dip Baked with spinach, Parmesan and mozzarella cheese.

Mozzarella alla Caprese Imported buffalo mozzarella, vine-ripened tomatoes, basil and balsamic vinaigrette.

Mushroom Ravioli Four ravioli stuffed with mushrooms and cheese. Served with our famous Carmela's marsala wine cream sauce.

Select one from the following:

Pasta

Penne Rustica Baked shrimp, grilled chicken, smoked prosciutto and penne pasta in a cheese sauce.

Pasta Milano Bowtie pasta, grilled chicken, sundried tomatoes and mushrooms in roasted garlic cream sauce.

Twice-Baked Lasagna with Meatballs Six baked layers of pasta with three cheeses and Bolognese sauce. Stuffed with meatballs and baked in our wood-burning oven.

Fettuccine Alfredo with Chicken Fettuccine pasta, cream, butter and Parmesan cheese with grilled chicken.

Chicken

Chicken Scaloppine Chicken breast, mushrooms, artichokes, capers & smoked prosciutto in lemon butter with pasta.

Chicken Parmesan Breaded chicken breast, tomato sauce, basil, mozzarella & Parmesan with pasta.

Chicken Portobello Grilled chicken breast topped with grilled Portobello, mozzarella and demi glace. Served with orzo pasta.

Seafood

Shrimp Portofino Shrimp, mushrooms, pine nuts, spinach & lemon butter with pasta.

Grilled Salmon Grilled salmon filet with a honey-teriyaki glaze. Served with spinach orzo pasta.

Desserts

Smothered Chocolate Cake Topped with homemade ganache and sprinkled with pecan pieces.

Tiramisu An Italian tradition of ladyfingers soaked in espresso liqueur, then layered between rich mascarpone cream.

Lemon Passion Citrus cake soaked in a sweet cream, topped with lemon mousse and finished off with our fresh Italian whipped cream and caramel.

Talk Abstracts

Alphabetical by Presenter

SAXS Data Handling at the ESRF: Current Situation and Future Prospects

Peter Boesecke and Claudio Ferrero

European Synchrotron Radiation Facility (ESRF), B.P. 220, F-38043 Grenoble cedex, France

boesecke@esrf.fr

Small angle X-ray scattering (SAXS) and related experimental methods, like anomalous SAXS (ASAXS), grazing incidence SAXS (GISAXS) and wide angle X-ray scattering (WAXS) are used on more and more beamlines at the European Synchrotron Radiation Facility (ESRF) in different scientific fields. However, a common strategy for processing data is currently not being undertaken, and is probably not even necessary in the present situation. In addition, there does not seem to be a strong users demand for it. The ESRF data format (EDF) is a commonly used internal exchange format, which is supported by the ESRF software groups and as such is easily portable between beamlines. However, its feature to save metadata and binary data in the same file is not always fully exploited. The common description is limited to the sizes of the images and of their pixels as well as the data type (integer, float, etc.). A general description of SAXS and WAXS metadata from pinhole cameras seems to be used only at the ESRF beamlines ID01 and ID02 (see ref. 1). The increasing demand for “fast” online data reduction can change this situation. During the last years the fast online correction program SPD, originally only used for SPatial Distortion corrections, has been extended to allow for basic SAXS data reduction. This program is now used by a host of ESRF beamlines, and not only SAXS beamlines. Depending on the beamline, the experimental data are distributed either in EDF format or in proprietary detector formats accompanied by log-files. Sometimes only 1D ASCII tables (q, I, standard deviation) of processed data are taken away by the users. The data are eventually backed up on movable hard disks or DVDs and carried along to the home labs. It should be mentioned that such a data backup is relatively cheap but not very safe.

The ESRF plans during the next years a major upgrade of the storage ring, the beamlines and the computing environment. The prospected higher photon flux will require faster detectors and faster analysis software. During time resolved experiments we are already now confronted with peak data rates in excess of 40 MBytes/s. We anticipate a significant increase in the future and a must of online data processing for most of the experiments. In order to cope effectively with the forthcoming challenges international collaborations (like the European FP7 project), the development of distributed computing (e.g. GRID), and the efforts to adopt internationally recognized data exchange formats (e.g. NEXUS) have been initiated.

References

1. P. Boesecke, Reduction of two-dimensional small- and wide angle X-ray scattering data, *J. Appl. Cryst,.* 40, s423-s427 (2007)

Small-Angle Scattering of Flexible Biopolymers

J. E. Curtis and S. Krueger

NIST Center for Neutron Research, NIST, 100 Bureau Drive, Gaithersburg, Maryland 20899, USA

Contact.joseph.curtis@nist.gov

We are developing a suite of computational methods to aide in the design and analysis of small angle scattering data with applications to macromolecular systems. This is achieved by generating an ensemble of macromolecular structures by varying sets of backbone dihedral angles and using mathematical methods to determine structures that have small angle scattering spectra that are consistent with experiment. We have used these tools to predict structures for the HIV-1 Gag protein under high salt conditions. The methods are applicable to the analysis of small-angle scattering spectra (X-ray or neutron) and can be applied to study intrinsically disordered proteins and other biopolymers in solution.

GRAS$_{ans}$P, D33 and parametric and complex data sets

C. D. Dewhurst

Institut Laue Langevin, 6 rue Jules Horowitz, 38042 Grenoble, France

dewhurst@ill.fr

GRAS$_{ans}$P and D33 are the two mistresses in my life. *GRAS$_{ans}$P* is Matlab™ based 'Graphical Reduction and Analysis Sans Program' particularly tailored for SANS data treatment of large, parametric or complex data sets. *GRAS$_{ans}$P* has been available for users of SANS instruments at ILL (France), PSI (Switzerland), NIST (USA), HMI (Germany), Juelich/Munich (Germany) and is distributed as both Matlab™ 'm-code' or as a stand alone, freely distributable compiled software package. The *GRAS$_{ans}$P* web site address is www.ill.fr/lss/grasp/.

D33 will be a third SANS instrument at the Institut Laue Langevin. Modern trends in materials science, physics and in particular nano-structured materials require that D33 should provide both high resolution and a wide dynamic range of measured scattering vector, q. In a 'monochromatic' mode a velocity selector and flexible system of inter-collimation apertures will define the neutron beam. A double chopper system will enable a 'time-of-flight' (TOF) mode of operation allowing an enhanced dynamic q-range (q_{max}/q_{min}) and flexible wavelength resolution. Two large multitube detectors will extend the dynamic q-range further giving q_{max}/q_{min} ~20 in monochromatic mode and a massive $q_{max}/q_{min} > 1000$ in TOF mode. Beam polarisation and ^{3}He spin analysis will facilitate and expand studies of magnetism and allow a more quantitative analysis of spin incoherent samples. The position of D33 will be such as to allow high magnetic fields at the sample position.

I will present examples of parametric data analysis using *GRAS$_{ans}$P* such as rocking curves or series measurements as a function of external parameters such as temperature, magnetic field etc. I will also highlight requirements for future data analysis with the advent of D33 such as parametric analysis and complex data sets from a SANS instrument working in TOF mode.

DANSE Software for SANS

M. Doucet, P. Butler

University of Tennessee, Department of Chemistry, Knoxville, TN

Contact: doucet@nist.gov

We will describe the current plans for the SANS group of the DANSE project. After going through the functionality we want to provide, we will present the release plan for DANSE applications. The structure of the code and the development process will also be discussed.

Insight Into the SANS Resolution and Instrumental Smearing

B. Hammouda and D.F.R. Mildner,

Center for Neutron Research, National Institute of Standards and Technology

100 Bureau Drive, Gaithersburg, MD 20899-6102

hammouda@nist.gov

Small-Angle Neutron Scattering (SANS) is a technique of choice for the characterization of nanoscale structures. This technique has grown to a sophisticated level with better instrumentation and advanced methods for data reduction and analysis. Desmearing of the data or smearing of the analysis models used to perform nonlinear least squares fits require detailed knowledge of the resolution function. The SANS resolution has been worked out in some detail [1-4] and will be presented for a number of cases corresponding to various instrumental conditions. The effect of gravity for long neutron wavelength and long flight paths will be discussed. Gravity modifies the iso-intensity contour plots from circular to elliptical close to the beamstop. Configurations that include neutron focusing refractive lenses and gravity correcting prisms will also be presented. Thorough formulation of the variance of the Q resolution and of the minimum scattering variable Q_{min} will be summarized.

References

1. D.F.R. Mildner and J.M. Carpenter, "Optimization of the Experimental Resolution for SAS", *J. Appl. Cryst*. 17, 249-256 (1984).

2. J.G. Barker and J.S. Pedersen, "Instrumental Smearing Effects in Radially Symmetric SANS by Numerical and Analytical Methods", *J. Appl. Cryst.* 28, 105-114 (1995).

3. D.F.R. Mildner, B. Hammouda and S.R. Kline, "A Refractive Focusing Lens System for SANS", *J. Appl. Cryst.* 38, 979-987 (2005).

4. B. Hammouda and D.F.R. Mildner, "SANS Resolution with Refractive Optics", *J. Appl. Cryst.* 40, 250-259 (2007).

Optimization and Minimization of Uncertainties in Time-of-Flight Small-angle Scattering Data Reduction

Rex P. Hjelm

Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

hjelm@lanl.gov

Data reduction procedures for the time-of-flight (TOF) small-angle neutron scattering (SANS) measurement should not mimic those that are used for data from monochromated sources. Rather, they should take into account the redundancy and quality of the data obtained from the TOF and spatial channels to meet the precision in differential cross section and Q needed for the experiment. This is particularly true, as current TOF-SANS instruments largely have fixed geometry and wavelength band-width; thus, the requirements in precision—except, obviously, counting times—are generally considered after the fact. Although the optimization rules for reduction of TOF-SANS data were formulated some time ago, [1,2] it appears that they have not been widely implemented. We will discuss these rules, their bases and the analysis of the instrument and source parameters required for their proper implementation. [3]

References

1. Hjelm, R.P., "Resolution of Time-of-Flight Low-Q Diffractometers: Instrumental, Data Acquisition and Reduction Factors", *Journal of Applied Crystallography*, **21**, 618-628 (1988).
2. Seeger, P.A., and Hjelm, R.P. "Small-angle Neutron Scattering at Pulsed Spallation Sources", *Journal of Applied Crystallography*, **24**, 467-478 (1991).
3. Olah, G.A. and Hjelm, R.P. "Analysis and Simulations of a Small-angle Neutron Scattering Instrument on a 1 MW Long Pulsed Spallation Source", *Journal of Neutron Research*, **6**, 79-93 (1997).

How to make code which will be compatible with Irena and Nika packages - programing user software in Igor Pro

Jan Ilavsky, Pete R. Jemian

Advanced Photon Source, Argonne national Laboratory, Argonne, IL, 60439, USA

ilavsky@aps.anl.gov

Igor Pro (Wavemetrics Inc., www.wavemetrics.com) is favorite platform for SAS data reduction and analysis software, utilized by number of institutions – for example NIST, IPNS, and number of APS beamlines. It's advantages are strong data processing combined with excellent graphic and data management capabilities – at reasonable price and with uniquely responsive support. Writing user code with complicated GUI is relatively easy and the code has very good cross platform compatibility between Windows and Mac OS X platforms.

Nika (http://usaxs.xor.aps.anl.gov/staff/ilavsky/nika.html) is package developed for reduction of 2-D data into 1-D lineouts for both small angle and wide angle scattering based on Igor Pro capabilities.

Irena (http://usaxs.xor.aps.anl.gov/staff/ilavsky/irena.html) package is large package combining number of SAS data analysis tools combined with utilities for data import, export, modification, and graphing. Other tools included are scattering contrast calculator for both X-ray and neutron scattering contrast, including Cromer-Liberman code for anomalous effects, desmearing routine (using Lake method) and various other useful routines. Both of these two packages (as well as Indra package for USAXS data reduction) are routinely updated and their functionality keeps growing as user requested features are added.

One of the challenges of programing user code in Igor is maintaining compatibility with other users code which may be included on their computers. Major issue for programmer is to make sure the name space and temporary space for each package is unique and does not conflict with other code, as these are shared. Some issues can be limited by good programing practices and are listed in Igor manual. Understanding of the programing principles used in Irena and Nika packages is helpful.

Second challenge is to help user in navigating through potentially massive amounts of data by using good and logical layout and by sharing the naming conventions.

This presentation will review basic rules and practices used in Irena and Nika packages, discuss existing data naming conventions and organization methods (and their advantages and disadvantages), and review available libraries which users can use to simplify their code and discuss available naming conventions.

SAXS and USAXS data format needs from APS point of view

Jan Ilavsky

Advanced Photon Source, Argonne national Laboratory, Argonne, IL, 60439, USA

ilavsky@aps.anl.gov

SAXS instruments present challenge for development of common SAS data format, as the variability of the instruments is probably larger than among SANS facilities. Cursory review of installed APS SAXS instruments showed, that no more than two share common area detector, resulting in wide range of different proprietary 2-D data formats used by detector manufacturers. Beamlines are often optimized for different applications and the control software is may be build on different systems. This results in complicated environment which is difficult to support.

As the data collection of synchrotron-based SAXS machines increases, number of pixels in 2-D image increases, and readouts of detectors improve (up to 30 Hz for "GE detector"), beamlines have to deal with humongous amounts of data collected in short time, which need to be reduced and processed. In some cases only dedicated software is capable dealing with reducing the 2-D data to 1-D lineouts for further processing. Organizing and maintaining integrity of the original image data as well as the reduced data is challenge. Most common 1-D data format at this time is a large quantity of ASCII data sets with reasonable naming conventions and folder organization. While this is cumbersome, it has unique compatibility with most of the available data analysis software.

USAXS instrument based on Bonse-Hart design presents slightly different challenge to data format, as often the data are slit smeared but with very high Q-resolution (fixed for all points). Ideally in case such the data should be modeled with models which include slit smearing. As the geometry of the Bonse-Hart camera is significantly different from pinhole cameras, not many parameters needed for data reduction and analysis are the same.

SAXS data analysis faces sometimes different considerations than when using SANS data. Wavelength of SAXS cameras is usually (not always) well defined by used monochromator so the wavelength spread smearing is unimportant. As the number of pixels of SAXS cameras is large the pixel size smearing can be sometimes neglected. On the other hand, commonly used program for 2-D data reduction, Fit2D, does not provide any error estimates and other packages ("Nika") provide errors which may not be sufficiently meaningful, which can pose challenge to data analysis software.

The presentation will review the needs of SAXS and USAXS instruments in view of development of common SAXS (1-D) data format.

Enabling software collaboration

A.J. Jackson[1,2], S.R. Kline[1], and P.D. Butler[1]

1. NIST Center for Neutron Research, Gaithersburg, MD 20899, USA

2. Dept. of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA

ajj@nist.gov

If collaboration on software projects is to be successful, access to the code and management of code changes is vital. Drawing on the example of the likes of sourceforge.net [1], the NIST SANS software team have built a software repository using Subversion [2] and Trac [3] to open up access to our code in order to enable collaboration with other facilities and with our user base.

In addition to the obvious benefits in terms of access to code, the use of Trac opens up the process of development to our users and allows them to comment on our development roadmap and submit bug reports. This transparency allows a more complete dialogue between users and coders enabling us to respond more easily to user feature requests whilst allowing users to see where the software is headed.

References

[1] http://www.sourceforge.net/

[2] http://subversion.tigris.org/

[2] http://trac.edgewall.org/

Embracing Dialects, But Speaking The Same Language

S.M. King

ISIS, STFC Rutherford Appleton Laboratory, Harwell Science & Innovation Campus, Didcot, OX11 0QX, UK

s.m.king@rl.ac.uk

Despite noble intentions, much consensus, a lot of fine words, and some hard work by a few individuals, nine years since the first canSAS meeting[1] the global SAS community *still* does not have a common format for one-dimensional reduced data, never mind 'image data'.

This talk will show that it is possible for the SAS community to share a common language – XML[2,3] – but nonetheless retain institutional dialects using a recent collaboration between ISIS-ILL-DLS as a case study.

References

1. http://www.ill.fr/lss/canSAS/postc.html

2. http://www.xml.org/

3. http://msdn2.microsoft.com/en-us/xml/default.aspx

An integrated e-Infrastructure for experimental Facilities

L. Lerusse, S.A. Sufi, K. Kleese van Dam, G. Drinkwater, T. A. N. Griffin, K. Shankland, D. W. Flannery, R. P. Tyer, , P. Couch, L. Blanshard

Science and Technology Facilities Council, e-Science Centre and ISIS, Daresbury and Rutherford Appleton Laboratories, UK

k.kleese@dl.ac.uk

The STFC e-Science Centre has built, in collaboration with STFC scientists, Facilities, and their users, an integrated e-Infrastructure, which enables the automatic capture, management, curation and exploitation of scientific data at scales ranging from Megabytes and minutes to Petabytes and decades. Jointly-agreed data and metadata standards allow data sharing between different facilities and Single-Sign-On facilitates cross-facility access for the users [5],[6]. This e-infrastructure has been deployed at the Diamond Light Source (DLS) and is currently in full operation at station I18 (Microfocus Spectroscopy), with more stations to follow. At ISIS, neutron data collected over the past 23 years of operation has been catalogued and made available to the users and new data will be automatically catalogued on existing instruments from late October 2007 onwards. A closely-related data collection infrastructure for the new Central Laser Facility 'Astra Gemini' project is also under way, with other related deployments planned for ISIS-TS2 and Lab-in-a-Cell. These developments are well integrated into other national and international activities through collaborations with SNS-ORNL, the ILL and the ESRF.

Building upon this infrastructure, scientists are able to analyse, visualise and interact with large volumes of scientific data from their desktop. This technology has facilitated a number of scientific advances, such as:

- Development of a new 3D heart model, to gain better anatomical information for use as the basis for realistic models of cardiac electrical and mechanical activities.
- Prediction of new crystal structures, including a new polymorph of piracetam [1], a drug licensed in the UK for the treatment of cortical myoclonus .
- Establishing how arsenic is taken up and held in the pyrite structure and the factors likely to lead to its release, in order to avoid contamination of drinking water extracted from man-made wells [2].
- Studying the ability of different mineral types to bind dioxin, making it possible to remove it safely from the environment, and how best to immobilise plutonium and high-level radioactive waste [3,4].
- The search for more cost-effective ways to catalytically produce hydrazine from nitrogen by identifying the best transition-metal / ligands combination and geometry for the transition metal catalysts.

The talk will introduce the infrastructure and present initial user responses.

References

[1] Nowell, H. & Price, S. L. Validation of a Search Technique for Crystal Structure Prediction of Flexible Molecules by Application to Piracetam. *Acta Crystallogr. B* **2005,** *61.,* 558-568.

[2] M Blanchard, K Wright, CRA Catlow, Arsenic incorporation into FeS_2 pyrite and its influence on dissolution: A DFT study, Geochim. Cosmochin. Acta, 2007, in press

[3] Atomistic simulations of resistance to amorphization by radiation damage. K Trachenko, MT Dove, E Artacho, IT Todorov and W Smith. *Physical Review B* **73**, art no 174207, 2006

[4] Simulation of radiation damage in gadolinium pyrochlores. IT Todorov, JA Purton, NL Allan and MT Dove. *Journal of Physics: Condensed Matter* **18**, 2217-2234, 2006

[5] G Drinkwater, K Kleese van Dam, S Sufi, R Tyer, L Blanshard, A Manandhar, M Doherty, K O'Neill, A Woolf, M Williams: *The CCLRC DataPortal*: All Hands meeting 2003, Nottingham, England, 02-04 Sep 2003

[6] S Sufi, B Matthews "CCLRC Scientific Metadata Model: Version 2" DL Technical Reports, DL-TR-2004-001 (2004)

Vector Resolution of a Lens-Based SANS Instrument

K.C. Littrell,

NSSD,Oak Ridge National Laboratory, One Bethel Valley Road. Oak Ridge, TN 37831-6393, USA

littrellkc@ornl.gov

The fundamental challenges for small-angle-neutron scattering (SANS) are increasing the useable flux so that good data can be obtained from more weakly-scattering samples, increasing the range of the measured momentum transfer magnitude Q particularly on the low end corresponding to scattering from larger structural components, and measuring the scattering curves with higher resolution so as to better be able to distinguish between competing models for explaining the data or better understand polydispersity. One method for achieving all of these goals is to use lenses focused at the detector as incident collimation. These have already been shown experimentally to simultaneously improve flux on sample, resolution and range for both isotropic and anisotropic scatterers. In this work, the previous results for a functional form for the resolution width for isotropic scatterers are extended to include anisotropic scaterers. As is the case for scalar Q, the contribution of the sample aperture to the resolution function essentially vanishes at the focusing wavelength. Below this wavelength the resolution of a focusing SANS instrument is better than that of a pinhole instrument with the same flight-path lengths and aperture and pixel size.

Generic Data Acquisition and Data Reduction at Diamond Light Source and the SRS

M. Malfois[1], F. Yuan[1], G. Mant[2], W. Helsby[2], N. Terrill[1]

1 Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 ODE, UK

2 Science & Technology Facilities Council, Daresbury Laboratory, Warrington, WA4 4AD, UK

Marc.Malfois@diamond.ac.uk

GDA (Generic Data Acquisition), jointly developed by the GDA group at Diamond Light Source and Daresbury Laboratory, uses a single framework with a similar look and feel across all the beamlines to reduce the learning curve of the users. Moreover, this single framework reduces maintenance effort. The software controls the Beamline devices, the sample environments and performs the data collection. Its main programming language is Java but a scripting language in Jython is also provided to the users. Its flexibility permits a customisable GUI and “plug and play” for new extensions based on new panels. The data reduction package used on I22 at Diamond Light Source was written independently of GDA and added as a “plug in” to GDA.

Dream (Data Reduction Easily Made) is the package that will carry out data reduction on line for both 1D and 2D data on I22. Building on the GDA software, we have developed simple data reduction screens that will take the users through the basic steps, data normalisation, detector response correction and experimental background subtraction. Working with live data from the current experiment and using only a few adjustable parameters, it will give a real time view of the data so that experimental decisions can be made during beamtime rather than later offline when it is too late to amend the experiments strategy. These simple mode screens are complimented by a scripting engine that will permit more complicated operations to be performed. It is planned to "pipe" the data from these programs into user community data analysis packages including FISH and all of those from CCP13.

What's hot and what's not? The essential features of reflectometry analysis software.

A.R.J Nelson

Bragg Institute, Australian Nuclear Science and Technology Organisation, New Illawarra Rd, Menai, Sydney, Australia

andrew.nelson@ansto.gov.au

Motofit is a neutron/Xray reflectometry analysis package that has been developed to meet most needs of beginning and advanced reflectometry users. It was created out of a frustration that most programs often lack the remaining parts that make them indispensable. For example, you can have a graphical user interface, but you can't refine multiple datasets. Or, you like the analysis, but you don't know how the program does what it does because it's a black box.

Here I describe the essential features of Motofit, it's strengths and weaknesses, as well as its possibilities for future extension. As an example I will present the Genetic Optimisation module, which is becoming widespread in reflectometry analysis, but is not as common in small-angle scattering software. This module allows the user to start with poor initial guesses for a model, yet still find the best fit available. Its ability to find a global minimum is essential for most scattering analysis, as some functions are topologically complex, made worse when fitting multiple contrast neutron and X-ray reflectometry data.

References

1. http://motofit.sourceforge.net
2. A. Nelson, "Co-refinement of multiple contrast neutron / X-ray reflectivity data using MOTOFIT", *Journal of Applied Crystallography*, 39, 273-276 (2006)
3. R. Storn and K. Price, "Differential Evolution - a simple and efficient scheme for global optimization over continuous spaces." TR-95-012-ICSI, (1995)

We've sorted out the data, now what was the sample again?

C. Neylon[1,2], J.G. Frey[2], A.J. Milsted[2] and J. Hale[2]

S.T.F.C. Rutherford Appleton Laboratory, Didcot, UK OX11 0QX,

School of Chemistry, University of Southampton, Highfield Southampton, UK SO17 1BJ,

C.Neylon@rl.ac.uk

Sharing and making available the raw data from experiments is becoming an increasingly important requirement for the scientific community. Government funding agencies are moving towards requiring open access to the results of publicly funded research and there is an increasing expectation that much more of the detail of experimental data will made available as supplementary information in the published literature. Standardised data formats can make experimental data from SAS experiments fully accessible to the interested community. However without access to minimal information on the sample this information can be of limited use. Details of sample concentration, monodispersity, and oligomerisation state are crucial in determining the reliability of conclusions made on the basis of the data. However, even where the scattering data is made publicly available or reported in the peer reviewed literature there is often limited information on sample preparation and characterisation made available.

We propose the meeting considers whether a minimal standard of reporting on samples should be adopted. If such a standard were adopted it could be applied either at the level of publication or at the level of facility access through a requirement for minimal reporting on samples. Applying a standard for publication could be achieved by adopting a community standard based approach similar to that used for the reporting of DNA microarray experiments. However this would only apply to published data. The advantages of mandating minimal sample description at the level of facility access is that all data would then be collected in one place and available for the future in a useful form allowing for re-analysis and re-use.

Recording data on sample preparation requires tools and standards and providing the data requires systems that can capture data and provide access on request. We are developing and using an electronic laboratory notebook based on a Blog format to capture experimental data in a biochemistry laboratory. Within the system each sample is recorded in a single post. Analysis and manipulations of the sample are recorded in separate posts with links back to the sample. All the information is made immediately available on the Web as it is recorded. Our objective is to capture all the relevant detail of our sample preparation and characterisation and to make this freely available, along with all the relevant experimental data, and any analysis of the data. While this approach will not be suitable for all disciplines, nor all scientists, it provides a model of how sample preparation data can be shared and made accessible for the future.

Probably the Last Word in 1D SAS Data Formats

R.E. Ghosh, S.M. King & A.R. Rennie

ILL, 6, rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France

ISIS, STFC Rutherford Appleton Laboratory, Harwell Science & Innovation Campus, Didcot, OX11 0QX, UK

Dept of Physics, Box 530, SE-751 21 Uppsala, Sweden

ghosh@ill.fr ; s.m.king@rl.ac.uk ; adrian.rennie@fysik.uu.se

Technology can now federate the innate tendencies of each SAS facility to develop its own data and software standards. Writing data in simple XML[1] format allows standard tools to interconvert from one structure to another, with appropriate changes in tag names. Increasing use of XML files in many aspects of GUI control and system layout ensures there will be continued tool development in the future. For the SAS community the XML file offers a man-readable and machine-treatable data form. Further extension to include data measured with a range of sample conditions in a single file comes as an obvious extension to the structured layout.

The sasCIF format specification of Svergun & Malfois[2] established a basic dictionary of terms, and provides a formal basis for archiving data, though it lacks structure for easy data extraction or manipulation. The NeXus raw data project evolved at much the same time, having an implicit structure from its roots in the Hierarchical Data File of the NCSA. The nomenclatures from the two approaches were compared[3]. We adopt a similar style to NeXus, though simplify presentation and parsing by proposing the clear inclusion of the units in the name of the metadata component rather than as a separate attribute to be parsed. Providing a four column table of scattering vector, intensity, and the experimental deviations of each, allows many instrumental parameters to be (optionally) omitted.

Many occasional users of the SAS technique will appreciate the ability to drop XML data into **Excel2003** (or later) and find the data automatically entered into the spreadsheet with labelled columns. For many packages, Java, Python, etc, there are library routines to parse XML. For traditionalists using Fortran, a C++ wrapper has been developed[4] for use with Frank van den Berghen's simple XML parser[5]. These routines can be easily adapted to other languages. The use is illustrated in a simple file converter for existing standard ILL data, using a dictionary of multiple aliases. Extension to parse local sections of multi-measurement files is straightforward.

References

1. http://www.xml.org/xml/resources_focus_beginnerguide.html

2. http://www.embl-hamburg.de/ExternalInfo/Research/Sax/reprints/sascif_2000.pdf

3. ftp://ftp.ill.fr/pub/cs/sans/can3king.pdf

4. http://www.ill.fr/lss/canSAS/forxml.htm

5. http://www.applied-mathematics.net/tools/xmlParser.html

FISH: The Friendly Face of SAS Data Model-Fitting

J. L. Rawle and R. K. Heenan

ISIS Facility and Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0QX, UK

Jonathan.Rawle@diamond.ac.uk

FISH is a powerful small-angle scattering data fitting program. It is best suited to the fitting of a curve with a large number of data points by a model with relatively few parameters. The built in models cover a wide range of possibilities including polydisperse spherical cores and multiple shells. Constraints may be applied and models combined and extended, making the possibilities of the program semi-infinite.

The program's previous text-based interface presented a steep learning curve for users. The new version features a graphical interface, making the software much more accessible, while retaining its power and flexibility. The graphics plotting routines have been replaced, and the plot now updates automatically as the fit progresses. Further planned enhancements include the ability to fit a series of datasets automatically and the ability to read and write standard data formats seamlessly without the need for conversion. The new interface is Java-based, making it cross-platform compatible, and leaving open the future possibility of integration with beamline data acquisition systems.

References

1. R. K. Heenan, *Rutherford Appleton Laboratory Report* RAL-89-129 (1989)

Thanks to our sponsors

NIST Center for Neutron Research

Argonne NATIONAL LABORATORY

LANSCE
Los Alamos Neutron Science Center

OAK RIDGE NATIONAL LABORATORY
NEUTRON SCIENCES