

Preamble

We'd like to thank all of you for your continued support of the NCNR. In particular, we very much appreciate that more than 450 of you took the time to fill out the survey conducted by our user group executive committee. We try to improve the NCNR every day so that it will continue to be an outstanding place for neutron-based research. Thus we were gratified to see that you feel that the NCNR has generally improved over the years. This was clear both from the trends of the individual categories and questions and from your responses to the "trend" questions. More details and graphs from the recent survey can be found on the user group web pages at: <http://www.indiana.edu/~lens/nug/nug.php>

It was also gratifying to learn that 37% of those contributing to the survey have in some way used CHRNS* education and outreach activities. It is clear that these activities help grow the neutron community. We will continue to focus our efforts on the most effective programs based on your responses, including the CHRNS* Summer School, travel support for first time users, online courses, and summer undergraduate research fellowships (SURF).

We were also happy that many of you took the time to submit comments. These were largely positive with one referring to the NCNR as "a national treasure". We very much appreciate these sentiments. We also greatly appreciate the many kind comments about our staff. We believe that the NCNR staff is outstanding and were quite pleased to see that you overwhelmingly agree.

We have now looked at the hundreds of comments in some detail trying to identify things that you would like to see changed at the NCNR. In doing this, we paid particular attention to those areas where the ratings were somewhat below the high bar set by the average scores and also to items where we believed we could provide insights into constraints we face or to how we see our priorities. After discussing this with your representatives on the NCNR User Group Executive Committee, we have developed a response/action plan that we will pursue to hopefully make your next visit to the NCNR even more scientifically productive and enjoyable. We should note that we do not intend to limit our actions to those which we highlight here.

As a final point, the NCNR User Group Executive Committee conducted and summarized the recent user survey. They have spent additional time providing constructive advice to help us improve the NCNR based both on the survey and on their own experiences at the NCNR. We thank them for their service.

* CHRNS is the Center for High Resolution Neutron Scattering which is a partnership between NSF and NIST which supports the operation of the NGB 30 m SANS instrument, uSANS, MACS, the backscattering instrument, and neutron spin echo spectrometers. This support includes sample environments, user laboratories, and ^3He spin filters for these instruments. Finally, CHRNS supports all education and outreach activities at the NCNR. The NSF contribution to CHRNS is funded by DMR-1508249.

Health Physics Training

Computer based training - too much information to be effective and is counterproductive.

Most of the content of the training we don't really get to make use of it. I think the computer based training could be shorter and tailored to the user's needs.

Compared to some other neutron and X-ray facilities the required training is a bit long.

It took hours longer than necessary.

Training prior to access was too slow. If training is necessary on site, it should be focused on the lab tour and quickly hit the highlights.

The updated training process is a HUGE improvement.

Being able to do training off site is great.

Moving the training online was very helpful.

The discussion of survey meters is too long.

We agree that the updated training is a big improvement. We also understand that users' time is very valuable and that our training often seems excessive, providing more information than is necessary for visiting researchers to safely perform their work. However, it is our responsibility - and a regulatory requirement - to cover all hazards and required topics for the entire area where the individual has access. To this end, our training program is periodically reviewed by the Nuclear Regulatory Commission to ensure that it meets this requirement. That said, we continually evaluate the content and make adjustments where appropriate and which are consistent with our training objectives. As part of this review, we remove content which is deemed redundant or unnecessary and we adjust questions in an attempt to ensure comprehension and avoid ambiguities. We welcome specific comments about our training and will make changes as appropriate – just send an e-mail to our user office (ncnraccess@nist.gov).

While much of the required content is accessible on-line and can be completed before coming to the NCNR, there is still some content that can only be covered on site, including the use of radiation survey meters. We have recently implemented a guide for the Health Physicists who conduct this training. We believe that this will partially address concerns about unbalanced time burdens that were raised in the survey. The one-on-one portion of the training should consistently take less than 20 minutes. If it takes longer than this, please alert your local contact and/or NCNR management.

Reindoctrination at 2 yrs is too often and very inconvenient for a 4-5 yr PhD

The frequency of our training is based on regulatory guidance, so changing this is unfortunately very difficult. We do note that our frequency is consistent with industry standards and that many facilities regulated by the Nuclear Regulatory Commission have annual rather than biannual training requirements.

Refresher training could be made more efficient by including less background and concentrating on safety and emergency signals/procedures.

Our refresher training is a trimmed down version of our initial radiation safety training. Only that content which has been deemed absolutely necessary for review has been included. We will review this material and determine if further narrowing of the scope is possible.

Beam time is precious and incoming users do not need to know about uranium-containing plates.

The issue of “uranium-containing plates” is likely due to a miscommunication on our part. The plates are a prop used for instruction in the proper use of survey instruments. The explanation of the radioactive content of the plates is merely a shared fun fact.

Proposal Process

Experience similar to other US user facilities

more stream-lined over time

I think it seems daunting for first time users.

It is very difficult and non-logical to register and propose a project.

Beamline scientists at the NCNR are very responsive and helpful when discussing proposed experiments and feasibility -- more so than other national laboratories in my experience

First-time access was fair, and the subsequent relationship with NCNR staff facilitated return visits.

Submission process has become much easier.

The clarity of the proposal form and the transparency of the review process remain high priorities of the NCNR. We recognize that first time users may find the process “daunting” and may need guidance in preparing successful proposals. We thus encourage users to work with an appropriate instrument scientist when writing proposals and planning experiments as they are eager to help. They will also help you register and submit a proposal. To further encourage this interaction, we will add a statement to that effect into the “Call for Proposals” email.

We are always working to identify potential reviewers with specific expertise. Thus, we welcome suggestions of potential reviewers. Please send an e-mail to our user office (ncnraccess@nist.gov) with any suggestions you may have. We are also placing a suggested reviewer box on the proposal which may be filled out at your discretion.

System for inputting materials/samples is very cumbersome.

We are aware that this can be an issue in many circumstances and have been discussing how to improve inputting of samples. As part of this process we have reviewed how this is done at other facilities. We also welcome any specific suggestions, just send an e-mail to our user office (ncnraccess@nist.gov). Hopefully we will come up with a new scheme that is much easier.

Instrument Control Software

I feel that ICE needs significant improvements, but with NICE being rolled out to the instruments soon, I think these will possibly be taken care of (ease of programming multiple runs, etc.)

BT7 data acquisition software (ICE) causes far too much overhead between data points.

Acquisition is very slow due to overhead in positioning equipment and checking setup.

ICP can be a challenge to start but once familiar, it is fine. Moving to new data acquisition makes it easier for new users.

Data acquisition software could be easier to use.

Software has improved but still slightly complex for more non-physicist backgrounds.

The new NICE software is fantastic.

The NICE software is easier to use and more intuitive.

Data acquisition software has been a significant issue for the NCNR. ICP is more than 25 years old, yet it is still running on four instruments. ICE is currently running on two of our newer instruments, BT7 and MACS. However, it has not worked nearly as well as we had hoped. Unfortunately, it is associated with substantial overhead and there are still occasional computer crashes. However, a recent “fix” involving the monochromator does reduce the overhead time for some scans.

To improve and modernize our data acquisition software, we are developing a new package called NICE. NICE is now running on NSE, the three reflectometers, the three SANS instruments, and the new test station (PHADES). NICE will also be the data acquisition software for the new instruments vSANS and CANDOR which will be rolled out in 2017 and early 2018. As these instruments are completed, we will turn our attention extending NICE to MACS and BT7. The user response to NICE has been generally favorable (see the comments above) and the instrument stability has been excellent. We are thus hopeful that NICE will be our data acquisition software for years to come.

Data Analysis and Visualization Software

I used Igor Pro with a Macro. It was really useful.

SANS control/reduction/analysis capabilities remain at cutting edge.

It would be better if IGOR were free

I use Steve Klein's Igor Pro macros for analysis, because as exciting as the new fitting engine is in SASView... SASView just cannot compete with the stability and interface of Igor. SASView has a LONG way to go until it is a usable piece of software.

SASView needs the ability to add custom models, it needs a much improved interface, and serious improvements in stability.

Data analysis is good to OK, depending on what instrument. I know they are working on this with SASView, but I find IRENA to be better.

I like what the APS offers to analyze USAXS data.

I used SASView and found that it is excellent for my purposes.

Refl1D is a significant advance, and keeps getting better.

Refl1D is the absolute best thing ever, hands down.

Data processing from data acquisition through reduction, to the analysis which yields physical insights is always of interest. Of that chain, data acquisition, reduction and visualization tools (such the Igor Pro reduction macros for SANS) are essential parts of each instrument. Thus with vSANS and CANDOR coming on line in the next 12-20 months, we are concentrating our resources towards producing reduction and visualization programs for these new instruments. That said, we believe that facilities have an essential role in analysis software. For years, the Igor Pro macros developed by Steve Kline have been an indispensable tool for fitting SANS data, but there are limitations imposed by the framework that bound possibilities for expansion.

SASView and Refl1D are open source programs that were developed as part of the DANSE project funded by NSF. Both have continued to improve, albeit slowly, since the project ended. SASView is now supported by an international collaboration with the routine participation of five neutron facilities (and others intermittently) albeit with minimal resources from each. Recently, the European Spallation Source (ESS) has assigned two people to work on SASView for the next two years, so we expect the rate of development to increase in the near term. Their priorities include improving stability, enhancing the

user interface, and incorporating a number of new models and enhanced analysis features from the SASfit package with the help of PSI and the SASfit author.

One of the recent improvements in SASView is the incorporation of the Refl1D fitting algorithm which is less susceptible to becoming trapped in local minima. It also provides more realistic error bars on fitted parameters than are obtained with a standard least squares approach. In addition, it provides a confidence interval in the real space scattering length density distribution and it allows users to visualize the correlations between parameters. We believe that the incorporation of these features into SASView is a significant advance.

Work has also been ongoing to make SASView and Refl1D run transparently on GPUs. This upgrade, which should be available in the next release, speeds up fits for reflectivity data significantly and will make fits of 2D SANS data practical, though they have long been possible in SASView.

One of the primary complaints about SASView has been the difficulty of adding user-defined scattering models. This issue was recently addressed and hopefully it will be more convenient to add your own function in the next release. The user interface has also been improved. Both SASView and Refl1D allow simultaneous fitting of neutron and x-ray data. For more information, see: <http://www.sasview.org/> and <https://pypi.python.org/pypi/refl1d> or contact Paul Kienzle (paul.kienzle@nist.gov).

Many users' analysis needs for SANS have grown far beyond traditional model fitting. Need to build more/better tools for: user-defined models, 2D/anisotropic models, data simulation (e.g. particle-based reverse Monte Carlo).

We agree that SANS data analysis needs to expand beyond traditional model fitting. While SASView provides some simple tools to obtain the pair distance distribution function and to simulate the scattering from a set of points with either magnetic or nuclear SLDs, more sophisticated real space techniques require new approaches which are more computationally intensive. To begin to address this issue, the NCNR is collaborating with an international NSF/EPSC funded project, CCP-SAS (www.ccpsas.org), which aims to reduce the barriers to using atomistic and coarse-grained modeling, to applying constraints based on as much *a priori* information as possible (connectivity, energetics, NMR, EM, etc.), and to exploring configuration space and identifying an ensemble of structures that are consistent with the scattering data. The project builds on SASSIE developed at NIST and uses GenApp to provide simple web interfaces and relatively transparent access to high performance computing resources. It also has an increasing set of computational modules to work with a growing number of problems. The public beta of SASSIE-web is currently available and will be refined over the coming year. For more information or to participate in the development of this software, contact Joseph Curtis or Paul Butler (joseph.curtis@nist.gov or paul.butler@nist.gov).

DAVE should be able to view and fit fp (Find Peak) scans. Should also be able to fit multiple data sets in PAN simultaneously.

DAVE is great. MSlice for MACS is excellent and supported very well.

Many of these features are present in DAVE, though they are not always obvious. For example, it is possible to view/fit Find Peak scans. Thus we can easily make this feature more prominent.

It is possible to convolute any user supplied instrumental broadening with any model function in the general purpose fitting routine, PAN. Fitting multiple datasets is done routinely by combining multiple

files into a single dataset with multiple groups. However, there is only limited support for making a surface fit where the model is a function of two independent variables. We are currently working to improve the functionality of the surface fitting option.

Data processing of time resolved data could be much improved, multiple file addition especially with time resolved data needs improvement.

real time data reduction for time resolved data

We appreciate that significant effort is still needed to properly streamline data processing for time resolved experiments using time-stamped data. At this point, our resources are concentrated on the completion of vSANS and CANDOR including full support for “standard” experiments. This work includes ensuring that the instrument and data acquisition software allow for time-resolved experiments using time stamping. In fact, the new data acquisition software NICE, supports time-stamping of the data on all instruments including the new instruments vSANS and CANDOR. However, it will be some time before we will be able to deploy the necessary resources to make data reduction and visualization for these experiments robust and easy to use.

Sample Environment

Additional cells that rotate to keep larger particles suspended during longer (SANS) measurements.

Rotating cells on the SANS lines

Temperature-controlled tumbling cell for BT-5 USANS

The tumbling cells that we currently have were built by Adrian Rennie from Uppsala University for a uSANS experiment and he graciously left them at NIST for other researchers to use. These cells have proven to be quite popular, though they did not allow for temperature control. We have developed a device to control the temperature above room temperature (up to 50°C with the parts in hand to upgrade to 80°C) and have utilized the device in an experiment. Other facilities are also actively working on developing temperature-controlled tumbling cells and we are monitoring their progress. The fabrication of additional cells and cells whose temperature can be controlled below room temperature will be informed by these developments.

More flow environments for SANS

Extensional rheoSANS, e-chem SANS

Electro rheology

Increase the stress limit (upper) for stress-controlled rheometer used for rheo-SANS

Rheometer and shear cell sometimes have issues

Need to document data reduction/correction scheme for more ... 1-2 and 1-3 plane rheo-SANS

The NCNR provides a variety of flow and shear devices for SANS measurements including two rheometers, a standard Couette geometry shear cell, and a 1-2 plane shear cell. The new set-up for making conductivity measurements at the same time as rheo-SANS is commissioning, and we believe it will be ready for general users soon. We have a new extensional flow cell than can be easily reconfigured to create a variety of flow fields. We are also actively working to create μ flow devices that can reach shear rates in excess of $10^6/s$ at temperatures as high as 200 °C for SANS. In all cases, software that can reduce the data in a straightforward way is an essential component of the

development. We will do our best to produce user-friendly software to both control the device and to reduce the data.

My one request might be a standard holder for SANS and USANS that will hold more samples at once. Especially on SANS there may be room for a second row of samples.

One of the most frequent requests we hear is for new temperature blocks for SANS that provide space for more samples as well as better temperature control to reduce the equilibration time. We are actively working to allow scientists to have the ability to control the temperature of individual samples or of a subset of the sample block rather than having the whole block at a single temperature. This would allow users to preset the temperature for the next sample and have it equilibrate while running a different sample.

Larger magnetic field at PBR (~3-4 T).

We have procured a 3 T superconducting magnet for PBR. It is a dry system with an open bore to accommodate a variety of different sample environments. It should arrive in the summer of 2016.

AC magnetic field generator

We have ordered an AC magnet for SANS that will produce a sinusoidal waveform field adjustable from 0 to 250 gauss and frequency from 0 to 10 kHz. The magnet will also cover 10 kHz to 20 kHz but with unspecified reduced field amplitude. The company building the magnet is now doing fit out and performance testing. We expect delivery in the summer of 2016.

Horizontal field SANS cryomagnet

Large bore cryomagnet for SANS with different field geometries/ directions

We have a 9 T horizontal-field, superconducting cryomagnet for SANS. We have had issues with this magnet over the years, and fixing it has been a low priority because it not in high demand. We are happy to report that it is currently working reasonably well. The minimum temperature is 2 K. For more information, please see: https://www.ncnr.nist.gov/equipment/NCNR_mags.html

We have no plans to procure another horizontal field magnet for SANS. One reason is that we cannot use a high-field horizontal magnet on the new vSANS instrument without impacting the NSE spectrometer. In the future, we may consider a vertical field magnet for vSANS as this configuration is less disruptive to NSE.

High pressure under very low temperature.

High pressure at ultra-low temperatures.

High pressure and low temperature <1K.

One must always remember that any facility cannot truly excel at everything and must set clear priorities for all aspects of instrument development and operations. Achieving the highest pressures available for neutron scattering is not a priority of the NCNR. That said, we do provide pressures up to 1 GPa using gas pressure cells. One of the advantages of these cells is that they can easily be placed in a top loading cryostat to provide the ability to continuously vary the temperature from 325 K down to <2 K. Achieving lower temperatures is problematic. We cannot put these cells in one of our dilution fridges

– it simply won't get cold. Thus the only possibility is to use a ^3He system and we only have one of these where it could be possible to achieve temperatures $<1\text{K}$ with our high-pressure gas cells. While we might try to do this, the dubious prospects for success at a reasonable capital expense will make it a "back-burner" effort.

Support Facilities

Most critical need is to be able to adjust samples off-beam between sequential measurements.

Increasing sample restrictions are beginning to affect functionality for some experiments.

We have had some trouble getting access/having space to work in the hot labs for sample manipulation after it had been in the beam.

The science being done (particularly on the SANS instruments) continues to evolve with many more samples now containing both organic components, which typically don't activate in the beam, and inorganic components which do. This activation means that any manipulation of the sample off line during the experiment must take place in the "hot" labs, which is quite inconvenient. To alleviate this issue, we will be building a new lab in the northwest corner of the guide hall. The design is complete and the construction contract is in place. We anticipate that this new lab will be available for users sometime in late 2017.

I suggest NCNR buy an X-ray Laue Machine.

We have purchased an X-Ray Laue machine for ex-situ orientation of single crystal samples. It is operational in the guide hall near the NG7 SANS instrument and immediately adjacent to the new neutron test station. The test station (PHADES) provides a monochromatic beam with a wavelength of 4.1 \AA which can be used to orient single crystals. More details can be found at:

<https://www.ncnr.nist.gov/instruments/instdev.html>

You may arrange access through your local contact.

Would like to see more/better analytical equipment for characterizing samples off the beam, particularly for fluids/soft matter (rheometer, DLS, etc.).

We have a wide variety of sample characterization equipment in our user labs. More details can be found here: <http://www.nist.gov/ncnr/laboratory-e136-sample-characterization-laboratory.cfm>

While the equipment is not top-of-the-line, it has the sophistication and functionality required by most users to characterize their sample before performing neutron scattering measurements. This equipment includes a DLS.

We have three rheometers that are used for SANS experiments. It is often possible to use these off-line. Please speak with your local contact.

NIST needs an FPLC for users to run a final gel filtration. They also need a Nanodrop spectrometer.

There is a nanodrop spectrometer on our "wish-list" of equipment. Each year, the scientific leadership of the NCNR ranks all items on the "wish-list" for inclusion on the next years spend plan as there are many more items that we would very much like to provide to our users and staff than our budget allows. In addition to equipment for the laboratories, this list includes small instrument upgrades (say a couple \$100k) and sample environment equipment. Please feel free to lobby any of the NCNR leadership to get your favorite item included or send an e-mail to Yamali Hernandez (yamali@nist.gov).

User Amenities

It would be more efficient if the network access code was sent to the guest users' emails a few days before the visit instead of going to the user's office and asking for one.

NIST is piloting open access to visitor wi-fi thereby eliminating the need for passwords. We believe that this service will be available at the NCNR sometime in 2017. In the meantime, wireless account passwords are e-mailed to all facility users. If a user submits a late registration, they can obtain their password either by visiting the NCNR User Office or by logging on to their IMS account on a visitor computer once they arrive. We have also received permission from NIST to text the password to users upon request after a suggestion by the NCNR User Group Executive Committee.

The wifi works much better now.

The use of internet among one's devices suffers when more than one device is online (e.g. laptop and cell phone)

We have been evaluating statistics on wireless usage in the user offices and have installed an additional three access points throughout the building. We will continue to monitor our visitor Wi-Fi to ensure that we have the necessary capacity to meet demand

... no visitor wifi in the guide hall...

The lack of visitor Wi-Fi in the guide hall is intentional to encourage users to leave posted radiation areas as an ALARA measure.

No phone reception in user office...

Phone access in much of the building is poor.

The user office weirdly has no cell reception. It is like the only room that doesn't either.

probably as a result of building design phone access in much of the building is poor. I don't know if there is anything that can be done about this, however.

Cell phone reception is certainly an issue at the NCNR. Our building has significant metal and other materials in the walls and ceilings that significantly reduce signal strength. NIST has assessed the feasibility of providing signal-boosting capabilities across the campus but various constraints posed by some carriers ended further consideration of that option. However, new technologies are becoming available all the time and we are actively lobbying to have the NCNR chosen to pilot a new approach to providing enhanced cell service at NIST. In the meantime, the new wi-fi access points should provide better reception for users with cell phones and networks that support wi-fi calling. In addition, line telephones are available in various locations within Building 235 and international calls can be supported on such lines in coordination with your local contact.

On a positive note, NIST has said that it will begin allowing the use of SKYPE on the visitor Wi-Fi network in 2017 so you will be able to make calls via the internet.

Desks in user office are usually fully reserved

The computer room is quite crowded. It would be nicer to have well-separated desks.

User office gets crowded at times

The NCNR has two user offices located in E115 and B100. The E115 location is often full or nearly full, while many of desks in B100 are typically not in use. Also, the desks in B100 are larger than those in E115. B100 is conveniently located for all thermal instruments including uSANS, as well as some guide hall instruments, particularly the NG7 reflectometer and SPINS. It is reasonably well-situated for NSE, the nSoft 10 m SANS instrument, and the CHRNS 30 m SANS although you must go over the catwalk. In the future, B100 will be a suitable office for the CANDOR reflectometer now being installed on NG1. On the downside, B100 is poorly located for access our user laboratories. If you believe that B100 would meet your needs for your next experiment at the NCNR, please feel free to mention it to your local contact.

... and I love the new coffee room.

I found the kitchenette last time I was there. It made for a much nicer 48 hours.

A lot of improvements can be made at break/snack room. Can we put some ready to eat (lunch/dinner pack) item on pay-as-you-use basis?

A vending machine with healthy options and even full hot meals should be considered.

My "fair" ratings relate to the fact that I was not aware of these user support facilities until my time at NCNR was almost over.

There was a snack room?

These varied comments (including those concerning user offices above) helped us realize that many users do not know the location of some of our amenities, such as the coffee room, coffee station, vending machines, and even the B100 user office. At the suggestion of the NCNR User Group Executive Committee, we have prepared a map of the NCNR highlighting these key areas. Copies of this map will be available in the user offices and in key places throughout our facility.

We are actively exploring expanding the food choices in the vending machines and have been for some time. After all we're at the NCNR every day and would like better food choices ourselves.

Unfortunately, the current NIST-wide food vendor refuses to provide fresh food items at the NCNR arguing limited demand and we are restricted in what we can do ourselves by the NIST contract with the food vendor.