The Neutron Advisory Board (NAB) met in Oak Ridge 25-26 May, 2015. Present were John Parise, Douglas Tobias, Meigan Aronson (chair), Robert Dimeo, Janos Kirz, Sunil Sinha, and Robert McGreevy, Jack Carpenter and Roger Pynn (ex officio). Not attending: Gabriel Aeppli, Frank Bates, Bernhard Keimer, Joel Mesot, Bill Sterling, John Helliwell, and Yujiro Ikeda.

The NAB was charged by the NScD to provide advice and feedback on the following issues during this meeting, and our overall impressions are summarized here.

Charge to the Neutron Advisory Board, February 2012

> Look at the "*Strategic Science Plan"* report, the "*Grand Challenge Workshop*" reports, the "*Instrumentation for Emerging Science: A Science Case for the Second Target Station (STS)*" report and the "*Technical Design Report*" and listen to our presentations on what next steps we plan to take to further engage the research community in defining a compelling science case for, and the technical and scientific characteristics of, the planned STS and advise us on the effectiveness of this plan.
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> Look at the "*Strategic Science Plan"* report and the "*2014 Instrument Health Pilot Project Procedures, Reports and Lessons Learned*" report and listen to our presentations on our path forward to maximizing the scientific productivity and impact at our current two neutron sources, HFIR and the SNS first target station, and advise us on the effectiveness of this plan.
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> Listen to presentations of new emerging science directions and areas of research and advise us if these ideas are going in the right direction and identify others that we should be pursuing.
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> Listen to presentations of our plan to increase science impact from neutron scattering through integration of computing and advise us on the effectiveness of this plan.

It is evident to the NAB that the science productivity and culture have made major steps in recent years. We especially enjoyed research talks from two most impressive young scientists. The fact that they were attracted to ORNL shows how positively the external world now regards opportunities at SNS/HFIR. We also note the increasing number of collaborations and interactions between NScD staff and other parts of the lab is becoming easier and more frequent, particularly in the area of novel materials and high performance computation. We observed that NScD management now has the bandwidth to do self-assessments, and is increasingly moving towards a decision making process for its activities and investments that is data driven and strategic. Management has successfully engaged the external research community in developing four Grand Challenge workshops, and are working to prioritize and implement exciting opportunities arising from the workshops, on both short and long time scales There is a palpable sense that real progress is being made, and that NScD is increasingly leaving behind the externally driven, reaction-based mode that characterizes operations of any successful construction project, and is transitioning into an organization with a distinctive voice and perspective. While the foundations of these accomplishments involved the dedicated efforts of many over the years, the new ALD and the members of his management team have ably taken up the challenge of continuing and accelerating this momentum.

Source Operations:

HFIR:

HFIR continues to operate with high reliability and for the planned 6 cycles per year. Within a relatively flat budget good progress has been made in arresting the decline of the fuel element inventory and the stock of critical spares. This demonstrates very careful management and should be commended. However, these issues will return if funding remains flat. Staffing remains a critical problem, with a significant proportion expected to retire within a few years. If key skills/knowledge are lost due to the (financial) inability to hire new staff for an overlap period then this takes a decade to recover. Possibly this can be addressed strategically at the laboratory level, since it must be a generic issue rather than particular to HFIR.

It should be discussed/investigated whether running longer cycles at lower power would benefit the science program, without being too detrimental to the isotope program or affecting the safety basis.

SNS:

The perception is that SNS operation has been dominated by the unexpected target failures. It must be stressed that, despite these events, the average availability is still excellent for a pulsed proton accelerator running at of order 1MW. The original anticipation was that targets might have to be replaced at the rate of 4 per year; the present rate has been 10 in 5 years. The target turn-round time of 10 days is impressive.

That being said, the bimodal distribution of target lifetimes strongly indicates a design/quality control problem. Since the high activity of used targets makes it extremely difficult to carry out detailed inspections, it is unfortunately necessary to make an educated guess as to the cause. The long lead time to target construction also slows the implementation of changes. The current approach has been detailed and thoughtful and has been independently reviewed. Both the surmised design issue and the cavitation issue are being addressed, including the use of He bubbles which looks promising from the tests at J-PARC.

For targets that have not failed the lifetime is determined by the criterion of 10 dpa irradiation, giving two target changes per year. This is somewhat conservative. We support the proposal to consider extending this (based on appropriate evidence and safety case) and moving to one planned change per year.

The reliability of the (60Hz 1MW pulsed proton) accelerator operation is impressive. While achieving the design specification of 1.4MW has been demonstrated and is an important goal for regular operation, it is only achieved by pushing the performance of several systems. This is a learning/development process (e.g. the work on in-situ plasma processing of cavities, which in itself is a significant achievement) and obviously increases the risk of unreliability if not properly managed. If the process is rushed the benefit for the science program (higher flux versus lower reliability) will show diminishing returns. We would therefore recommend that performance targets are set to demonstrate steady progress to the goal. An appropriately managed process is more likely to achieve success both for 1.4MW at the FTS and for the future power upgrade and STS. We support the view that attempting regular 1.4 MW operation before the planned installation and appropriate commissioning of the new RFQ is likely to be counter productive.

Some education of the external community as to the impact of various types of unreliability on the science program would be advised. This should include the rationale of aiming for one target change per year (if the decision is made). Probably 5% of the unreliability is short timescale faults that literally make no difference to the program and would perhaps be more appropriate to report as a lower average power. Longer outages can largely be mitigated by rescheduling affected experiments quickly. Most disruptive are 0.5-2 day outages, which are few.

Instrument Health Program

This is a very positive development aimed at providing a systematic basis for resource allocations aimed at improving instrument productivity and capabilities. We commend NScD management for launching this effort and enthusiastically recommend that it be completed as soon as possible and repeated at intervals. We urge NScD to expand the current Pilot Program as soon as possible to include all the SNS and HFIR instruments, as well as sample environment and also instrument software. Having all this information will make it possible to draw high level conclusions and – as intended- to inform decisions regarding key investments.

The decision to devote $10M to these investments annually is most laudable, and is an important signal that NScD is committed to the continuous improvement of its instruments, enhancing their ability to produce more and better scientific results. However, we are concerned with what was represented as a joint function of this program: enhancing existing instruments as well as initial funding for brand new instruments. Experience at other sources indicates that ~100$K per instrument is needed for maintenance in steady state. The remaining 2/3 of the 10M$ does not provide sufficient funds to make modest improvements in the instruments and also develop new instruments without external funding. We believe that the funds should be focused on making improvements to existing instruments.

There is something of an introspective flavor to the way that the information is gathered, in that it depends so heavily on input from the instrument scientists. There could be substantial benefit to including other voices, more along the lines of DOE reviews of beamline and instrument reviews. It seems problematic to not include users directly, perhaps as members of the review team.

Making priorities among many compelling options will be challenging, but we were impressed with the sincerity and seriousness of the management team in their focus on making decisions that will best balance the needs and opportunities at SNS and HFIR, particularly as they pertain to optimizing the three-neutron-source facility that is envisaged at Oak Ridge. We share their concerns that there is a real temptation to address simple and expedient improvements, but that this may not lead to the most strategic outcome. The Instrumentation Health Program is an impressive achievement, as it brings project management thinking and follow-through to investments and capital projects. How do you think of investments in SNS vs HFIR? Basic and reliable functionality vs capabilities that will be used by few but which rely on the special features of the source and instrument? Which instruments are truly world leading and which are workhorses responsible for solid scientific productivity? Considering these issues and coming to some working guidelines is perhaps the most important next step. We were impressed by the view that we heard that these upgraded capabilities and the resulting science are the foundations for a 1B$ investment in future. This strategic mindset should provide a certain degree of focus choosing among different compelling options. It is hard to see how the instrument health plan could be successful without the accompanying development of a working scientific vision that informs priorities. We feel that the current management team has members who are well able to do this. Perhaps it will be appropriate to appoint a small group to mine the completed instrument health report, in view of these directorate guidelines.

Meanwhile, we offer some specific observations on the Instrument Health Pilot Program:
Overall:
Add to the list of possible metrics 1.2.2 Capability, a bullet “Recognition of instrument problems and intended solutions.”

Powgen:
Shame on the supplier of the new scintillator plates!
Replace the present windows, 5 mm thick with new ones even thinner than the 1.5 mm thickness mentioned in the under the sample vessel replacement heading. Such thick widows not only reduce the available neutron intensity and introduce undesirable structure in the incident beam spectrum, but also contribute to the general radiation background. Most similar installations use membrane windows fractions of mm thick, which are deformed under hydrostatic pressure to the desired curvature and annealed before installation. The technology for forming such membrane windows was developed at SNS about five years ago; we are surprised to find that their use is not already widespread in SNS. Stop using safety as an excuse not to carry out this and other instruments.
Be more realistic about hydrogen gas management. Stop being scared of hydrogen, as the impact statement for POWGEN notes.

ARCS
In the process of replacing guides sections 3, 4, and 5, replace the aluminum windows with thin-wall membrane windows as mentioned above in relation to POWGEN.
Under the category Additional To Chopper, with the intent to reduce background 500-1000 microseconds after the prompt pulse (probably skyshine), be aware that the source of this background is probably NOT in the direct beam. *Check whether that background really can be stopped by blocking the beam.* Do this before committing to design, build and install another To chopper.
Under the Ideas for improved productivity from new users, do create a targeted school as the report recommends. *Periodically, dedicate some instrument time for this training*.
Under Vacuum systems, *ASAP do carry out the “long-planned but stalled ARCS and SEQUOIA vacuum systems upgrade*.

LESSONS LEARNED

Table 1 almost certainly must be corrected. The entry for SNS high impact publications is 45%!

From Grand Challenge Workshops to Enabling New Science

The Science Workshops that were held over the past year in various areas from Quantum Condensed Matter to Biomaterials, appear to have been very productive in generating scientific ideas for future exploration with neutrons from the scientific community. We were glad to see that the findings from these workshops are being assimilated by the scientists in the Neutron Sciences Division. The science workshops have identified compelling first experiments for the STS and in-depth analyses of the fields. In some cases, they have already stimulated preliminary experiments, and new instrument concepts, such as VENUS on FTS. Thus we applaud Alan Tennant's scheme of rating some of the ideas arising from these workshops into a 1-2-3 scheme based on strategic alignment, planning and prioritization, and areas of significant potential. It is clear that further work needs to be done by the scientific management team to fully absorb and plan for some of this potentially new science and to plan for the right expertise and ancillary equipment, and then to develop, and implement plans and priorities. The long-term health of the neutron facilities at ORNL will depend critically on their ability to deliver on "killer apps" and science that will be transformational and also address societal needs.

Increasing User Involvement

NScD has organized a number of recent workshops seeking input from the scientific community to identify grand challenges that can be addressed by neutrons. Other workshops have looked at various aspects of instrumentation and computing. The NAB recognizes and fully supports these outreach efforts – they have been an integral and important part of the planning process. Nevertheless, there appears to be a need to more fully engage the broader neutron user community in all aspects of planning. We noted, for example, the absence of a user representative at the NAB meeting itself which could be seen either as a sign of user apathy or of user exclusion. Whatever the explanation, the message sent by this absence is not a positive one. We did not see a clearly articulated strategy to fully develop user support for the three-source strategy, for strategic science directions and for new instrumentation at the STS as well as the two existing sources. In some instances, for example in enhancing software, the NAB suspects that users might articulate a somewhat different set of priorities to those presented to the NAB. If this is indeed the case, the various views will need to be integrated into a coherent strategy which users can and do fully support. It will always be true that the staff at ORNL have a more complete view of the possibilities that can be realized by new neutron instrumentation, techniques and source development etc. However, there is a need to make sure that this potential is fully communicated to the broader community so that the latter becomes an integral part of progress made at the facility as well as a cheering section for future development and funding. A coherent strategy for user engagement that involves staff at all levels within NScD would be a useful addition. One concrete suggestion made by the NAB is to inform users of NScD's interest in developing joint proposals for funding of exploratory research that would test novel ideas for science and instrumentation. Examples would include uses of very cold neutrons, neutron focusing methods, special purpose sample environments, etc.

Scientific Productivity:

The NAB is pleased by the overall increase in the number of publications making use of ORNL neutron facilities in the past 4-5 years. Nevertheless, there is a general perception that the scientific productivity on the NSD needs to increase. The number of publications has increased between 2012 and 2014 by about 20%, but the number of high impact publications has not, according to the data provided to the NAB.

What should be the goal for 2017? The report by the ALD indicated that there were 345 publications in 2014, and the goal of 400 publications in 2015 seems reasonable. The bigger questions are: What is a reasonable/aggressive degree of growth? Do we know how publications scale with beam intensity, number of instruments and their maturity?

A comparative analysis with the productivity of peer facilities – already started as part of the Instrument Health program, - seems appropriate, taking into account the relative costs of operation, the number on instruments in the user program, and other relevant factors.

To the extent that this is not already routine procedure, the NAB recommends that the NScD look carefully at the way general user proposals are evaluated, so that the ones most likely to result in high impact science, that use special features of the ORNL research environment, or that demonstrate new instrumental capabilities are given priority. In this regard it may be helpful to examine best practices at other BES facilities.

Development Opportunities: Making the Most of New and Existing Instruments

Time focusing

Geometric arrangements (locations, orientations) of source, sample, analyzer crystals, and detectors in crystal analyzer and other instrument can eliminate some of the effects of finite sizes upon resolution and provide higher intensities. Some simple implementations of these principles are in common use in TOSCA, VISION, and in standard setups for moderator emission-time measurements. But the general ideas have more-intricate implications, as explored for Crystal Analyzer Spectrometers (CASs) in computer studies by Zsigmond and Carpenter about 10 years ago, but never tested in prototype.

Because there may be good use for these principles in STS CASs, we suggest that time-focusing be examined in conceptual designs for STS instruments.

Coded Apertures

Use of coded apertures is already established in astronomy and other fields. The principle is a method of multiplexing the use of imaging applications by viewing the object through a multi-aperture mask with special mathematical relationships among the apertures of the array. The scrambled image is recovered by deconvoluting the recorded image using the inverse of the encoding mask; the encoding mask is often its own inverse.

There is almost certainly use of coded apertures in STS imaging applications; this is already done in some laboratories. And there is possible use of coded apertures in VULCAN-type instruments to increase the throughput and the field of view. We recommend that STS imaging instrument designers consider this multiplexing application. And to consider methods of producing the required masks, perhaps by material addition (3-D printing) methods, which is a challenging task for neutron applications.

Multiple Converging Aperture (MCA) Collimation

Small-Angle Scattering is conventionally carried out using double-pinhole or single-channel collimation that defines a single beam of radiation. In an arrangement in which many similar, separated channels define beams incident on the sample that converge at the detector, each position on the detector corresponds to the same angle of deflection, independent of which channel defined the individual beam. Such an arrangement can produce a compact instrument advantageous especially in time-of-flight applications in which there is a premium on short flight paths to increase the wavelength and Q-ranges.

The SANS instruments at IPNS accomplished this using pairs of converging Soller collimators, one with vertical slits, the other with horizontal slits, converging at the detector. A similar MCA is installed at Orpheé TPA SANS instrument, consisting of a converging series of perforated absorber disks, a “pepperpot” collimator.

We recommend that SANS instrument designers consider this option for time-of-flight SANS instruments at both FTS and STS. The required collimator might be made by 3-D printing of various materials. Robocast, Albuquerque, produced a prototype of Al_2O_3-Gd_2O_3, consisting of
9x9, 2-mm-square apertures, 1.5 inches long.

We also find it disappointing that there is this still no low temperature, polarized beam SANS capability, although this is currently available at NIST. As well, the sample can used at low temperatures is unnecessarily thick, leading to an unacceptably large background.

Scintillator Materials

Launch a program, with new direction, to oversee a neutron detector development program. Especially dedicated to new scintillation media. Priorities are efficiency, speed, and light output (which directly relates to resolution in pixellated detectors.)

Coarsely Pixellated Scintillation Detectors

There is need for coarsely pixellated (1 cmX5 cm), individual-channel, fast, efficient detectors, which should not be challenging to provide.

Very Cold Neutron Source

That is, ~3 °K Maxwellian spectra. [Cooling is the only way to increase the phase space density.]

First thing, determine whether there is appropriate space in STS to accommodate a VCN source; almost certainly, because the moderator needs to be 1-2 m from the target. Given that, proceed with technical assessment.

Computing Strategy

Data analysis, visualization, supplemented by modeling and simulation are key ingredients to maximizing the value of neutron scattering experiments. Over the years the NAB has urged that software development remain a priority to the NScD. Continuing developments in this area are critical to increased productivity, impact, and, ultimately, user satisfaction. There has been substantial progress, on both the hardware and software fronts, in data acquisition and reduction that have improved the user experience, and the NAB supports plans to upgrade the data acquisition system and change the workflow to enable data analysis to be done “on the fly” while an experiment is in progress rather than at the users’ home institutions. The NAB noted that VISION stands out as a shining example in this respect, since initial work suggests the performance and productivity that are expected of a world-class instrument at a 1 MW source.

The utmost priority should be rapid access to properly normalized datasets, which are absolutely essential for planning the progress of an experiment, and are prerequisite for further analysis, and for validating the results of modeling and simulation. The NAB has the impression that the quality of data analysis software is uneven across the suite of instruments at the SNS, and recommends that it be raised to a uniform, high level across the facility, immediately. To this end, software developers must communicate directly with instrument scientists and users, and be responsive to their needs, and software quality should be considered a key “vital sign” in the assessment of an instrument’s health. The NAB continues to support the development of the Mantid platform, in collaboration with other sources, for data reduction and visualization.

Productivity gains may indeed result from shifting more analysis from users’ home institutions to real-time visualization at the neutron facilities. However, the NAB is concerned that many practical problems need to be solved to bring computational advances to the user level. Without engaging the user community and understanding their needs, scarce resources may not be optimally allocated. The basic assumption is that users will be expert enough to carry out their own analysis and this is really an obstacle to productivity, especially for inexperienced users. These users could profit from focused software support and they could bring new ideas.

Given the collocation of NScD with the leadership-class computing facilities in the CCSD at ORNL, it is natural for NScD to take advantage of the outstanding computational resources, infrastructure, and the expertise of CCSD personnel, as exemplified via CADES, CAMM, ACUMEN, and the data science pilot project. As presented to the NAB, this aspect of the computing strategy at NScD is a research project, with major components that may not be capable of delivering dividends to a broad user community, are impractical in the near term, and are likely to be unsustainable. The goal of enabling users to carry out molecular dynamics simulations to assist data interpretation while an experiment is in progress is a much discussed dream; the presented calculations of phonon dispersion curves during a HYSPEC experiment is an impressive example of what is possible. However, this accomplishment was only possible because the user had modeling expertise and access to a supercomputer during the experiment. To fully realize the dream for the broader user community, presumably a team of modelers would need to be present to assist users, and dedicated computer resources would need to be available; it is conceivable that providing such capabilities would double the cost of operating an instrument. If such a path is to be followed, it will require sustainable funding beyond the initial investment of a pilot project. This prompts the question: how far should a neutron facility extend its reach into the simulation enterprise? A possible solution would be to launch a targeted program of joint PhDs, which would bring long term benefits with respect to engaging external user groups and developing the software innovators of the future.

The NAB strongly recommends that the computing strategy not be dominated by "over the horizon" initiatives; there are plenty of important problems that need to be addressed today to increase productivity and the quality of the user experience. Overall, the NAB had the impression that users are not playing a big enough role in shaping the computing strategy within NScD.

The Three Source Complex at ORNL

The three-source complex is an integral part of the unifying vision for neutron scattering at ORNL.

The vision for neutron scattering at ORNL fundamentally includes HFIR, FTS, and STS. The combination of the three sources permits all the benefits enabled with a continuous, high flux source at HFIR, short, sharp pulses at FTS, and short, long wavelength pulses permitting a larger dynamic measurement range at STS.

A comprehensive, coherent communications plan should be developed that articulates the three-source vision to staff, users, and sponsors.

It is not enough to develop this three-source strategy as part of the unifying vision for neutron scattering at ORNL. It is equally important to communicate this strategy effectively to the staff, users, and sponsors. The staff should understand the vision of the three-source complex first because (1) they have a vested interest in being a part of a vibrant complex for neutron scattering, and (2) they communicate directly with the neutron users. The users must understand the strategy because they continue to rely on ORNL to provide current and future capabilities as part of the US neutron measurement infrastructure and they have a vested interest in the developments in neutron science at ORNL. Finally, the Department of Energy's Office of Science must understand this strategy of a three-source complex because it will provide the maximum scientific output for the investment.

The NAB recommends that ORNL-NScD develop a comprehensive, coherent communications plan that describes the compelling case for a three-source complex at ORNL in which each of the three sources is considered an integral part of the whole. This should be reflected, for example, in presentations and other types of communications to staff, users, and stakeholders.

There have been numerous compelling arguments made that describe the broad benefits of the science that is carried out (or will be carried out in the case of STS) at each of these facilities. These will not be repeated here. However it is important to understand that the whole of the three sources at ORNL will be greater than the sum of its parts. Optimization of instrument capabilities at any individual facility is a key to maximizing its scientific productivity. The optimization benefits grow if you have more than one source because there are more degrees of freedom to explore in the optimization. For example, relocating an instrument from one beamline to another beamline with better beam characteristics for that particular measurement type not only increases the impact of that instrument but it also provides an opportunity to install an instrument at the vacant spot better suited for the beam characteristics at that location. This endeavor is cost-prohibitive at a single source, and in some cases even technically impossible. Thus it enables a cost-effective way to maximize the collective scientific productivity and impact of the sources.

Deciding Among Compelling Opportunities

It is clear that the NScD is developing a process in which they plan to take a corporate-level approach to prioritization. They presented a number of the important elements of that process. One that the NAB heartily endorses is the Instrument Health Program for assessing the strengths and weaknesses of the current instrument suite. Progress and success towards realizing the three-source complex at ORNL mandates the adoption of a more comprehensive decision making process by the NScD team that is informed by data and by performance characteristics and of other relevant criteria that will maximize scientific productivity of the three-source complex. We think as well that there is need to develop and clearly articulate a scientific vision that could be used by NScD management and staff as a structure to guide future decisions.

We enjoyed our 2015 meeting in the Clinch River Cabin, which has a very pleasant and inspiring setting that is conducive to good discussion. We were somewhat under full force this year, and so we ask that the NScD continue to organize future meetings at least 6 months in advance. This will permit all NAB members to attend the meeting, and also will allow a more systematic and interactive development of the meeting agenda and charge to the NAB, so that the meeting can be maximally useful and efficient.

We want to thank Jeanine Evans in particular for her work in making the meeting so successful, and also for the excellent catering that brought out the best efforts of all participants.