Workshop on Long-Pulse Neutron Instrumentation

Background and Philosophy

The European community is currently working to develop plans for the ESS, a 5 MW long-pulse spallation neutron source, and the SNS in the US is currently developing plans for a second target station (STS) operating in the long-pulse mode at ~1 MW. Therefore it makes sense for the US and European communities to pool resources to develop a better understanding of what might be possible with neutron beam instrumentation optimized for operation at high-power long-pulse spallation neutron sources.

Since both the ESS and the STS are in the early conceptual design stage, there is currently considerable freedom to tailor the neutronic performance of each of these sources by varying the target-moderator-reflector geometries and materials to optimize the performance of the neutron beam instrumentation to meet the scientific goals (likely somewhat different at each facility). It has been demonstrated that such neutronic optimization can lead to large gains provided it is appropriately matched to the requirements of the associated instrumentation (a striking example is the ISIS Second Target Station). Therefore, it is timely to carry out a systematic process of instrument optimization to define the source performance parameters best suited for particular instrumentation, so this information can be fed back into the source design process.

There are at least two different ways to approach such a systematic process of instrument optimization. One way is to select a set of important scientific problems and then look at how to design instrumentation to meet the requirements for each of these problems. An alternate approach is to note that advances beyond the capabilities of current sources and instrumentation generally require improvements in some combination of the following four areas:

- Smaller samples (access to new materials existing only in small quantities)
- Faster measurements (kinetic processes, non-equilibrium systems, parametric processes)
- Larger length scales (biology, soft-matter chemistry, aggregation, self-assembly, vortex lattices)
- Longer time scales (big floppy systems)

One can thus systematically look at how far each measurement technique can be pushed in terms of the four broad areas indicated above (e.g., How far can you push SANS in the direction of small samples or of rapid measurements or in length scale?), and then pick and choose which technique or combination of techniques could be used to achieve a specific scientific goal.

The recent long-pulse instrumentation workshops in Europe (Rencurel, 2006 and Ven, 2008) and the STS instrumentation workshop in the US (Oak Ridge, 2007) as well as several much earlier long-pulse workshops have all been more along the lines of the second alternative, but none of these has systematically looked at how to optimize instruments and source characteristics to push these limits.

In order to really understand how well an instrument will work for a specific scientific problem, one needs to simulate (or otherwise evaluate) its performance with a realistic model for the sample of interest (or at least a simplified model sample matching the required range, resolution, sample size, type of measurements desired, and other parameters important to the science in question) and then evaluate how well the information of interest can be extracted from the simulated data. It is not practical to do this for every interesting scientific problem and for every sample of interest. However, modern instruments at pulsed sources are capable of generating huge amounts of data covering different energy and momentum transfer ranges and often also with widely varying resolutions. A meaningful evaluation of instrument performance must include an assessment of how much of this data is useful, and this will require at least a few such simulations of real samples and scientific problems of interest. Thus the ideal systematic study probably includes a marriage of the two different approaches to optimization indicated above.

Optimization and assessment of instrument design concepts should also take into account practical factors such as instrument cost, practicality of really long beamlines, limitations due to beamline crowding close to the moderators, etc.. The optimization process should also be designed to point out potential source modifications to enhance the instrument performance.

Workshop Goals

1. Systematically extend the understanding of the strengths and weaknesses of various types of long-pulse-source instrumentation optimized to address differing types of scientific problems, and how far this instrumentation at the proposed new sources could surpass current capabilities. Particular emphasis is to be placed on extension of current capabilities in the direction of smaller samples, faster measurements, larger length scales, and longer time scales as indicated above. It probably will not be possible to carry out all the simulations necessary to complete this process during the course of this workshop, but it will be important to take advantage of the large body of instrumentation expertise that will be present at the workshop to develop instrument concepts thought to be appropriate to the specified scientific problems, and at least to specify in some detail the simulation(s) required to evaluate and/or optimize these concepts.
2. Develop innovative new instrumentation approaches to address some of the weaknesses found in conventional instrumentation approaches.
3. Utilize the instrument optimization process to identify source modifications and/or new component development that would significantly enhance the instrument performance.
4. Develop plan for longer-term coordination of activities to further extend these systematic studies, including provisions for carrying out the simulations suggested by, but not carried out at, this workshop , and provisions for developing the analysis software that may be required to extract the information of interest from the simulated data.

Workshop Plan

The workshop will be held August 26-28 at the Villa Mondragone (lodging in nearby Villa Tuscolana). The Villa Tuscolana will be reserved for a couple more days after the workshop in case the simulators or others wish to remain to implement some of the simulations or to address other instrumentation issues that could not be addressed during the workshop (similar to what was done after the Ven workshop).

The workshop will start with a short plenary session addressing workshop organization, goals, logistics, etc. There will also be one or two short plenary sessions to report working group status during the course of the workshop, and a longer plenary session to close out the workshop with reports of working group results and discussion future plans.

However, most of the workshop would be devoted to working groups, broken out along the lines of particular types of instrumentation. The success of the workshop will be dependent on having a strong leader for each of these working groups to ensure the work proceeds efficiently to meet the workshop goals. These working group topics will be:

- Diffraction and imaging, including single-crystal diffraction; powder, total scattering, liquids diffraction; engineering diffraction; and imaging
- SANS and USANS
- Reflectometry
- Larmor techniques including spin-echo
- Direct geometry and inverted geometry inelastic scattering

Relevant reading material will be made available to workshop participants prior to the workshop.

Each working group should address the questions of how far that type of instrumentation can be pushed in the four areas indicated above (smaller samples, faster measurements, longer length scale, longer time scale), or if warranted, how far the instrumentation can be pushed in other areas that may be relevant. To provide focus, each instrument design and optimization should be carried out to address a specific scientific problem, preferably one from a suggested set of scientific problems developed prior to the workshop. If it seems appropriate for addressing a particular problem, two or more working groups can combine or can share experts for part of the time. Also, it is anticipated that some of these working groups will break up into sub-groups to address different sub-topics for some of the time. Movement of participants between working groups is also encouraged.

Instrument design concepts should take into account practical factors such as instrument cost, practicality of really long beamlines, limitations due to beamline crowding close to the moderators, etc. The optimization process should also indicate any potential source modifications (e.g., different spectrum options, different length of long pulse) that could enhance the instrument performance.

Although not the primary goal of this particular workshop, working groups are also encouraged to identify other areas where development could significantly enhance instrument performance (e.g., specific component requirements, analysis software, etc.). Some of these might profitably form the bases for focused future workshops and/or for specific R&D at individual laboratories.

Each working group should contain or have access to the instrumentation experts and simulators as appropriate to address the stated workshop goals. In addition to the working group members there need to be several floating “devil’s advocates” to challenge the groups. There should also be source neutronics experts representing the ESS and STS sources to interact with and get feedback from the working groups.

The goal would be for each working group to develop during the course of the workshop instrument concepts for as many of these combinations of scientific problems and areas where better performance is required as possible, and to define the simulations desired (including instrument concept, bounding requirements, and questions to be answered). Time permitting, implementation of some of these simulations could also be carried out. A further goal would be to develop a plan for carrying out the remainder of this work after the workshop.

Each working group would be expected to provide status reports during the course of the workshop, and to produce a written report (to be compiled into an overall workshop report) shortly after the workshop.