REPORT FROM IU SANS ANALYSIS MEETING
July 24-25, 2008

Indiana University Cyclotron Facility hosted a discussion group on July 24-25, 2008 to discuss the SANS analysis need of LENS and ORNL, the SANS analysis landscape at present, and the opportunities for the future, in the context of the DANSE project and the new instruments coming on line.

Participating in the discussion were:

> Paul Sokol, LENS
> Helmut Kaiser, LENS
> Dobrin Bossev, LENS
> Paul Butler, NIST and DANSE
> Mathieu Doucet, DANSE
> Greg Smith, ORNL Large scale structures
> Ken Littrell, HFIR SANS
> Josh Pierson, SNS EQSANS
> William Heller, HFIR BIO SANS
> Steve Miller, ORNL Data handling group
> Michael Reuter, ORNL Data handling group
> Jean Bilheux, ORNL Data handling group

The group began by discussing standard data formats. The need for standard formats was agreed to be absolutely critical. It was noted that the canSAS working group had in fact recently finalized its standard reduced 1D formats which both NIST and HFIR representatives said they were committed to supporting (and ISIS had already begun to implement). It was agreed that DANSE should support this format. Further it was recommended that a standard 2D format be agreed upon soon. There was some discussion of the NeXUS format but in the absence of a finalized standard no further recommendation was made by the group.

The current emphasis of the overall DANSE project on developing web apps and virtual instruments was thought to be completely inappropriate by this group, at least as far as the SANS community is concerned. Due to the high degree of visualization and interactivity, portal access to standalone applications or web services based applications would be a higher priority. In that vein the group discussed priorities both in terms of philosophy and in terms of the prioritization of new functionalities. With respect to philosophy, the group noted that there are two parts to bringing in new science: providing new functionality (helping expert users do more), and making current functionality more accessible (helping to develop the novice user base and helping the more established user become more productive). The group suggested, that for DANSE to succeed it needed to begin to cultivate a user base ASAP and that it should focus first on making current functionality more accessible. The HFIR representatives indicated that if DANSE was easy to install and use and included all the current NIST IGOR analysis functionality,

plus the 2D analysis of SliceView, and transparent handling of parametric data, they would adopt it as their standard package. Representatives of LENS and SNS indicated that the NIST functionality would be sufficient for them to begin the adoption noting that SliceView has already been installed and usable at SNS for a while now. The NIST representative indicated NIST would begin migration once the DANSE application became equivalent in functionality and ease of use to its current package. NIST further indicated that it looked forward to the opportunity to be able to focus more efforts on its acquisition and reduction and only participate in, rather than be the sole provider of, the analysis software. The DANSE group indicated they expected that their alpha release of the first DANSE SANS application, due in January of 2009, would contain most, if not all, the models available in the current NIST IGOR package.

The group noted the existence of a number of packages that provide standard analysis and suggested that the canSAS plan to provide a central SAS portal should move forward posthaste and should not only provide a list of available packages, but some idea about their appropriateness for specific areas, their language, origin, user base, and, if possible, an honest critique on ease of use, correctness etc. The group also made a quick list of new SANS functionalities that would be useful and prioritized them as follows:

1) 2D analysis.
2) Transparent handling of parametric data.
3) Transparent use of a variety of optimization algorithms and the ability to simultaneously fit data from different sources (including techniques) where the parameters of the models for the different sets can be related through some function.
4) Simulations of inelastic, and multiple scattering effects particularly for TOF data where a variety of wavelengths contribute to any given q point.
5) 3D rendering/visualization of models used in analysis whether or not used by a simulation.
6) Transparent use of distributed computing.

It is interesting to note that with these 6 items, the group suggested that virtual instruments be number 11 in priority and that web apps be 12.