Meeting on ESS instrument simulations at NBI 25/11/10

Present: Ken Andersen, Kim Lefmann, Peter Willendrup, Emmanuel Farhi, Klaus Lieutenant, Uwe Filges, …

Manpower situation:

There are roughly 6 full-time equivalents in Copenhagen for ESS instrument simulation.

At HZB, there will be 2 people for 3 years working under Klaus.

At ESS in Lund, the first instrument scientists will start in 2011: Hanna Wacklin (reflectometry) in January, Pascale Deen (cold-neutron spectroscopy) in February, someone for powder diffraction in April, hopefully someone for spin-echo around July. A SANS position is being prepared, and another 4 instrument-scientist positions will be advertised in 2011, probably TAS, Protein crystallography, Imaging, backscattering.

Kim presented the work on optimizing a strawman instrument suite as a function of accelerator time structure. This work was presented to the ESS SAC in November. The higher-frequency, longer-pulse-length part of the performance table needs to be filled out for completeness, which will be done. The results will be published in NIMA.

Ken presented the technical boundary conditions from the accelerator side and a rough analysis of the calculated instrument performance. The performance scales roughly as the peak flux, with the time-integrated flux being less important, leading us to favour the highest peak flux allowed by the accelerator. This is limited by the 50mA peak current of the ion source, recommended by the accelerator scientists.

The instrument list arrived at by the SAC had been expanded to 22 instruments (day one plus day two). Kim pointed out an error for the 10mmeV BS instrument, which needs to view a thermal source, not cold.

The instruments fall into 3 distinct length groupings: short (up to 35m), 100m and 200m, resulting in three “guide halls”. A possible layout was presented.

We then went through the list of instrument simulation wishes from the ESS SAC (ESSSAC\_wishes\_Nov10\_KL.doc). Main comments are noted below.

Powder diffraction:

The first objective is to simulate a real diffractogram on GEM with a reference sample. We need a good description of GEM, which already exists (from Klaus?) The simulated data then need to be treated in the same way as real data, for example using Mantid. Work is already well underway to integrate McStas with Mantid: McStas can write Nexus files. Mantid reads them and reduces the data.

The GEM model will then serve as a baseline for the ESS instruments to be simulated: 200m narrow-bandwidth TOF, Multi-monochromator D20-like, shorter GEM-like multi-RRM instrument. Of particular interest is how to merge data sets taken with different chopper phases or to provide a single diffractogram from slewing the choppers. As for the simulated GEM data, the virtual data must be treated in the same way as real data and then Rietveld-refined. The performance metric is the refinement quality.

This work should be coordinated by the ESS powder-diffraction instrument scientist, who will hopefully be spending a few weeks in Copenhagen/Lund in February to start this activity. Kim & Peter to distribute the work in Copenhagen.

Protein crystallography:

To optimize this instrument, we need good advice from Paul Langan, with whom Peter is already in contact. A visit to LANSCE may be a good idea. Start by playing with divergence and instrument length, under the supervision of the ESS powder-diffraction instrument scientist. SAC suggested a 70m instrument with RRM. A 140m instrument with no RRM may work better.

Cold single-crystal diffraction:

This is lower priority than the thermal powder diffraction instrument. The aim is to combine D7 and D10 capabilities.

Bi-spectral extraction:

About a 1/3 of all the instruments would like to have a bispectral source. We need to study how we can accommodate a large number of beams next to each other, all with their own supermirror switch. Kim & Peter to distribute the work in Copenhagen. Klaus brought up the idea that if we have a water premoderator between the cold moderator and the target, we could perhaps use the spectrum from the premoderator for the bispectral extraction. We need to have a better idea of the moderator geometry. Ken to get reasonable geometry numbers from the ESS target-moderator group.

SPES Engineering diffractometer (Kampmann/Schreyer) will be looked at by GKSS, with support from Klaus.

SANS & Reflectometers:

Uwe Filges informed that at PSI they are performing tests of the Selene concept which will be very useful for the ESS instrument evaluation. They will also measure the amount of off-specular scattering from a supermirror and inform the Copenhagen team for integration into McStas. Using MCNP, they will estimate the background for both the very short SANS instrument and the Selene reflectometer. This is a critical issue for the very short instruments. Hanna Wacklin will be coordinating the reflectometry work after she arrives in January. It is important to examine several instrument concepts and compare. The SANS instrument scientist position is about to be advertised. The person will probably be in place in the second half of 2011.

Cold-neutron spectroscopy:

We need to reexamine the comparison between IN5-type and TAS-type instruments. Look at different types of samples: Low-dimensional crystal where data can be integrated along a certain Q-direction, real 3D crystal where we are interested in only a fairly small part of Q-w space. Optimising for small or bigger samples or sample-environment which restricts the solid angle. The performance metric will depend on the science. Several different scenarios should be prepared. This work can probably wait until we have a TAS-type scientist at ESS.

Imaging:

We need to make good use of the expertise where it exists: TUM, PSI, HZB

Sources:

Ken will send Kim & Peter the SNS source data he got from Melissa Sharp. Peter and Klaus will send Ken the brightness curves from Vitess and McStas source components for the various existing neutron source. Ken has brightness curves for ILL, J-PARC and the ISIS TS1 H2 moderator. Ken will produce reference brightness curves for as many neutron facilities as possible. Some of the numbers from Paolo Radaelli’s Expert Meeting diffraction report do not seem reasonable, but we cannot at the moment judge them quantitatively.

Guides:

Elliptical guides provide good transport over long distances, good focusing at the sample and a uniform divergence distribution. You probably cannot do much better on these three criteria with any other geometry. However, the problem of eliminating direct line-of-sight for gammas and fast neutrons is still not solved. Curved guides may be the best solution providing only a small degradation in performance compared to the elliptical guides. The combination of parabolic expansion, parallel-sided curved guide and parabolic refocusing needs to be looked at in detail: transport efficiency, wavelength-dependence, spot size, divergence uniformity, etc. We also need to look at how well we can transport shorter wavelengths (down to about 1Å seems reasonable). I seem to remember that this work was delegated to Kaspar Klenø, but that is for Kim & Peter to decide on.

Target monolith geometries:

We need something like 0.5m separation between the axes of adjacent pulse-shapingS choppers. If they are at 6m, that gives an angular separation of 5 degrees. At 100m the instruments are separated by 8m. At 200m they are separated by 15m. LET has 3.5m L2, giving a total instrument diameter of at least 10m. 15m instrument separation is not crazy.

5 degree separation between all beams would allow 240/5 = 48 instruments. This assumes we can use Fermi choppers for pulse-shaping. Big disk or T0 choppers need 1.5-2m between beam axes. You could almost get there by having every alternate choppers above and below the beam axis. It would help also if the beams alternated between above and below the target.

We might also be able to increase the total instrument fan above 240 degrees: If the proton beam comes from below, we might be able to increase the angular coverage in the backward direction.

It is also possible that we can have a thinner monolith in the backward direction: 4m forward, 6m backward may be sufficient.

We need to look at whether it’s possible to have PS choppers inside the monolith.

Ken to coordinate the work with the target group and ensure that we get critical input

Closed meeting:

An ESS user meeting is planned for the day after ECNS. Ken will check with Jan Saroun if the planned simulation meeting is still going ahead and arrange with him how to deal with a potential conflict of dates. ESS could look into helping with him with their venue for the Sunday.

We agreed that, as a general rule, a completed instrument optimization should result in a short report. Peter will set up a repository of ESS simulation reports on [www.esss.dk](http://www.esss.dk) = [www.ess-scandinavia.dk](http://www.ess-scandinavia.dk) which can be referenced in publications. PDFs of publications could also be placed there, but would need to be password-protected to avoid copyright problems.

Kim will arrange to have the last few sections of the Ven paper written. A draft of the SANS section could be written by Klaus for Albrecht to work on.

The time-structure paper will be written up for NIMA. Ken will write a draft of a summary section for that.

Next meeting: 16/12 starting at 14:00 with a dinner planned after.