Minutes of ESS simulation meeting 25/11-2010

KLe and KHA, 3/12-2010

<u>Participants</u>

ESS:	Ken Andersen
Copenhagen:	Stig Skelboe, Kim Lefmann, Anette Vickery, Kaspar Klenø, Jonas Okkels Birk, Johan Jacobsen, Sonja Holm, Morten Sales, Linda Udby (observer: Klas Risveden)
Risø-DTU:	Peter Willendrup, Britt Rosendahl Hansen, Lars von Moos
HZB:	Klaus Lieutenant, Heloisa Bordallo
PSI:	Uwe Filges
ILL:	(observer: Emmanuel Farhi)

(Excused: Erik Knudsen, Esben Klinkby, Morten Sales, observers: Mogens Christensen and Niels Bech Christensen)

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0. The team

Emmanuel Farhi (EF) has joined as an observer from ILL, and is highly welcomed in the group. Klaus Lieutenant (KLi) has has recently moved to Helmholz-Zentrum Berlin. Uwe Filges (UF) from PSI is still participating in the project. Ken Andersen (KHA) has been employed by ESS to chair the instrumentation developments and is in this respect our closest collaborator and “customer”.

At Risø-DTU, Britt Rosenlund Hansen (BRH) has been employed as a post doc. The Risø team is still lead by Peter Willendrup (PKW) and counts further Erik Bergbäck Knudsen (EBK) and Lars von Moos (LvM). Roughly 2 FTE (full time equivalents)

At Univ. Copenhagen, the computing efforts are led by Stig Skelboe (SS), with Lars Melwyn (LM) as system responsible for the computer cluster. In the simulation group Anette Vickery (AV) has been employed as a post doc, while Johan Jacobsen (JJ) has joined as a master thesis student. Heloisa Nunes Bordallo (HNB) has been employed by the ESS to be stationed in Copenhagen from 1/3-11; she will participate in the simulation efforts. The simulation work is led by Kim Lefmann (Kle). The group further counts Kaspar Hewitt Klenø (KHK), Linda Udby (LU), Esben Klinkby (EB), Jonas Okkels Birk (JOB), Sonja Lindahl Holm (SLH), and Morten Sales (MS). 5 FTE.

1. The situation

1a. Time structure

KLe presented the simulations efforts on time structure, which involved simulating 16 very preliminary instrument models over 17 different accelerator time structures (pulse length and frequency). The outcome of this study is that the effective use of neutrons increases strongly with shorter pulse and lower frequency, in particular the figure-of-merit scales as the peak flux to a power of 0.7 (for constant time-integrated flux). This was presented to ESS-SAC by KHA in November 2010.

KHA presented the technological boundary conditions from the accelerator group showing that the accelerator power will be limited by the peak current (50 mA), which therefore points towards longer pulse and higher pulse frequency to keep ESS competitive in terms of neutron production, i.e. to reach 5 MW power, while shielding etc. will be designed to allow 10 MW of power. It is foreseen that the pulse length will be 2 ms, although this is not fully decided until spring 2011.

The discussion of a hot spot on the moderator has been put on hold until the target/moderator people are ready to discuss this. However, it is clear that all instruments would benefit from this.

It was decided that the remaining 3 entries (the corner with long pulse, short repetition rate) should be filled into the figure-of-merit table for all 16 instruments. This work will then be published in NIMA (Nucl. Instr. Meth. Section A).

1b. Manpower and collaborations

The Danish group has increased by 4 persons, to reach 7 FTE, as indicated above.

In Germany, a large effort (21 M€) is starting in 2011. KLi will hire 2 post docs at HZB, and also GKSS, FZJ, and FRM-2 will enter the instrumentation and simulation work. It will be important to coordinate this large effort so that we benefit fully from the large increase in manpower.

ESS is hiring instrument responsibles, which will be the central points of coordination for the instrumentation work. Hanna Wacklin covers reflectometers and will start 1/1-11. Pascale Deen covers cold spectrometers and starts 1/2-11, while a powder diffractionist will start around 1/4-11. SANS and spin-echo will be covered in summer 2011, while crystal analyzer spectrometers, protein crystal diffraction, imaging, and backscattering will be filled later.

Coordination and information will be a problem. We must immediately fill information into the simulation web page (managed by PKW). Wiki lies at www.esss.dk, but perhaps we should have an "outside window". Downloaded publications should certainly be password protected.

1c. Meetings

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

2. Priorities and distribution of future tasks

KHA presented the destilled outcome of the ESS experts meeting and the ESS-SAC meeting as a list of 22 instruments (20 instruments, if different versions are considered as one). KLe had a few corrections: the TOF-TAS instrument should be considered both as cold and thermal, probably two different instruments, and the 10 μeV backscatter instrument should be thermal.

As a general observation, about 1/3 of the instrument are below 50 meters and could be placed in a hall close to the source. 1/3 of the instruments are around 180 meters or more and could be placed in a distant hall, which would cover around 30 degrees of angular view of the source. 1/3 are intermediate length instruments and could be placed in a third hall, covering around 40 degrees of view. The idea of beam extraction and/or guide bundles should still be considered, in particular for the intermediate length instruments and for beamlines for testing, optics, and crystal alignment.

In a common discussion, quite a number of open questions were identified, to be answered by simulations. Below, these are divided into two general questions on guide systems and description of sources – and questions related to each of the 21 instruments: 7 diffractometers, 4 large-scale structure instruments, 8 spectrometers, and 2 imaging stations. The time horizon for the priorities below is 6-12 months, as the situation can change rapidly.

This should be seen in connection with the note by KLe on the SAC priorities, dated 10/11-2010.

Source descriptions:

We must compile descriptions from contacts at the sources and make use of what is already available in McStas and VITESS. KHA will forward data from SNS, ILL, J-PARC, and ISIS TS1. PKW and KLi forward tabelized data on sources to KHA.

Guide systems: 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 up to 200 m (down to about 1Å).

A number of other guide issues should be investigated:

- Wavyness of guides, effect on the intensity in the center of the beam.
- Parabolic guides with curvature – also in the presence of hot spot in the moderator.
- Guide bundle, e.g. two instruments use same pulse shaping chopper.

A testcase for most of this could be the bispectral magnetism diffractometer.

Target monolith geometries: We need around 0.5 m separation between the axes of adjacent pulse-shaping choppers. If they are at 6 m, the angular separation will be 5 degrees. At 100 m the instruments are separated by 8 m. At 200 m they are separated by 15 m. LET has a secondary flight length of 3.5 m, giving a total instrument diameter of at least 10 m. Therefore, 15 m instrument separation is reasonable for similar-length instruments.
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 1.5-2 m 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: 4 m / 6 m may be sufficient.
We need to look at the possibility to have pulse-shaping choppers inside the monolith. KHA will coordinate the work with the target group and ensure that we get critical input.

Thermal powder diffractometer, narrow bandwidth: The requirements for this instrument is short wavelength (below 1Å) and good wavelength resolution (dl/l). This does not come naturally for a long-pulsed source. However, for scientific reasons, ESS must have at least one powder diffraction instrument, even though it will not be an order of magnitude better than ISIS/ILL instruments. A number of instrument designs should be tested, all of which have a resolution chopper, with a few additional constraints:

- The GEM type instrument with a large wavelength band (50m) and RRM.
- The Vaals “angular dispersive” instrument of 180-200m length and no RRM.
- For the instruments it should be checked if a vertically focusing guide could be used – and the height of the detectors should correspondingly be reduced (scattering plane instrument). This idea must be credited to Leo Cussen.
- The test of the diffractometers will be to perform Rietveld refinement of merged virtual data (or simultaneous fit of unmerged data). This is difficult and we must work with a crystallographer. We would then need to simulate the detectors also, and incoporate MANTID capability into McStas. EF notes that the (u,v,w) formalism may not be correct.
- First: simulate virtual data from existing GEM instrument, and compare to real data. KLi may have a GEM model.

KLe and PKW will distribute the tasks for thermal powder diffraction.

Thermal powder diffractometer, general purpose, GEM type:

(see description above)

Hybrid thermal powder diffractometer:

This is a multi-monochromator instrument, D20 like, where the time structure is used to separate wavelengths. Idea from EF and (perhaps independently) somewhere in SAC.

Cold/magnetic powder diffractometer:

The description of this instrument is expanded to cover the wavelength range 2-6 Å, i.e. a mixture of D7 and D10 at ILL. We could use this instrument as a test case for the parabolic-curved-parabolic guide, perhaps with guide splitter. Or beam stop early in an elliptic guide.

This instrument is also a test case for the bi-spectral guide, does it perform well with elliptical/parabolic guides? KHA will obtain geometry information from the ESS target-moderator group. We should investigate how this works with a bright spot on the moderator(s).

This simulation has a lower priority than the thermal powder, but is still on the SAC day-1 list.

Protein crystallography:

This instrument has fallen a little behind in the simulations until now, and there is a strong need to investigate a number of designs. The ESS SAC says 70 m and RRM, but we should also investigate longer (100 m RRM or 180 m with/without pulse shaping).

We need to get input from a number of protein crystallographers. We start with Paul Langan, Sine Larsen, Garry McIntyre, Dean Myles, and (someone at FRM-2). We may need to visit LANSCE.

Extreme conditions diffractometer:

(this diffractometer is on the list, but was not discussed)

Engineering diffractometer:

The starting point is the GKSS design, SPES, by Kampmann and Schreyer. It must be foreseen that GKSS will take over this design and simulation with assistance from KLi. There is a German meeting about this in December 2010.

Short SANS:

The simulations of the basic optics of this instrument are sufficient – we will double-check with experts, e.g. Lise Arleth.

UF will calculate the background for such a short instrument, using MCNPX.

Long SANS:

(see description above)

Vertical reflectometer:

It should be checked if the reflectometers are too close to the source with respect to resolution and background (see short SANS). We should also check if SELENE is a good idea for pulsed sources. We must also address the issue of off-specular scattering from supermirror guides. PSI will look into this and perform experiments to feed back into McStas. Several instrument concepts must be tested.

It could be envisaged to hold a dedicated reflectometer meeting. There is a German meeting in January. We should not work on this project until then. It could be envisaged that these simulations will be performed by our German and Swiss colleagues.

Horizontal reflectometer:

(see comments above)

Cold chopper spectrometer:

We have a good model for the spectrometer, including RRM. We should include also pulse shaping chopper, and consider going to 180 m. We must test flux numbers against existing spectrometers, e.g. CNSC, IN5, LET. Toby Perring has vanadium-data (for LET) and Jacques Ollivier has for IN5.

We should compare this instrument to cold TAS and cold TOFTAS by virtual experiments for two cases: a) low-dimensional magnet, b) 3D system where a small part in (q,w) space is important. We should also investigate small/large samples.

Thermal chopper spectrometer:

This spectrometer must be 180-200 m long and use a pulse shaping chopper. The pulsing chopper at sample must be a Fermi chopper.

Compare to other spectrometer types: thermal HYSPEC-type spectrometer (simulate that also), thermal TAS (we have model). Compare to IN4.

Cold TOFTAS:

This should be 100 m long. This spectrometer is being simulated at NBI in collaboration with EPFL. Test scattering from all material, using Mcstas multiple scattering (collaborate with EF). Consider bi-spectral.

Must compare with IN14 and IN20 flat cone with Si(111). Also compare with TAS and cold chopper at ESS. With/without magnet.

Thermal TOFTAS:

180 m long, pulse shaping chopper. See also comments under cold TOFTAS. Compare to HYSPEC-type and thermal chopper at ESS. With/without magnet.

Cold backscatter spectrometer:

180-500 m long. Si (111). Test 1.5 μeV to 3 μeV resolution. Compare to BASIS, OSIRIS, and IN16.

Thermal backscatter spectrometer:

Use Si (311) analyzer. 10 μeV resolution. 180-300 m. Pulse shaping chopper. Used mostly for pure elastic scattering at high Q.

Classical spin echo:

Most important is high spin-echo times. Wait until the instrument responsible is in place.

Wide-angle spin echo:

Wait until instrument responsible is in place.

High flux imaging station:

German and Swiss specialists are setting up a working group. Meeting in Germany next spring. We foresee that this instrument is taken care of by German and Swiss groups.

High resolution imaging station:

(see comments above)

Fundamental physics beamline:

We await closer information from the community.

The present distribution of simulators on the simulation tasks is given in the table below:

Task	Other	KLi	UF	EF	PKW	EBK	BRH	LvM	KLe	AV	KHK	JOB	JJ	SLH	MS	?
*** Sources ***		x		x	x											
*** Guides ***		x	x								x			x		
*** Monolith ***	KHA															
Th powder, BW																?
Th. powder, gen.															x	?
Hybrid th powder																?
Cold powder		x							x		x			x		
Ex. cond. diffract.					x		x									
Protein crystall.					x		x									
Engineering diff.	GKSS	x														
Short SANS			x						x		x					
Long SANS			x						x		x					
Vertical reflect.	PSI	x	x					x								
Horizont. reflect.	PSI	x	x													
Cold chop spect.									x	x	x					
Th. chop spect.									x	x	x					
Cold TOFTAS									x			x	x			
Thermal TOFTAS									x			x	x			
Cold backscatter									x		x					
Th. backscatter									x		x					
Classical NSE						x										?
WASP NSE																?
Imaging, flux		x	x													
Imaging, resol.		x	x													

3. Documentation and publications

General statement: Everything should appear on the repository at www.esss.dk. We should write papers on what is significant.

3a. Reports

KLe reminded that all work must be documented and appear on the home page. It was agreed that each instrument would be documented in a full report (e.g. 6-8 pages), to give more information than the one-page standard sheet. Both should appear on the home page.

From the minutes of the March 2010 meeting:

"The reports will all be written in LaTex and will have the standard sections

1. Introduction (e.g. which type of instrument is simulated)
2. Earlier work (both design studies and simulations)
3. Instrument design (including effect of modified pulse parameters)
4. Simulation results (including figure-of-merit)
5. Conclusion (including suggested pulse parameters for this instrument)"

3b. Journal articles

Time structure paper is first priority, must submit fast! KHA writes a section on the accelerator details and summary. KLe adds 1-2 examples. One-pagers as URL. To be sent to NIMA.

The Ven paper has second priority. EF approches Wiedenmann, otherwise KLi writes about SANS. KLe will finish thermal spectrometer section.

KHA will comment on guide report from KHK in view of a publication or two.

Next Meeting

Will be held 16 December, 14.00 at HCØ. We will have a neutron dinner in the evening.