

Minutes of ESS simulation meeting 20/4-11

KLe, 24/4-11

Participants

ESS Science: Ken Holst Andersen, Richard Hall-Wilton, Hanna Wacklin, Paul Henry, Marie-Louise Anaheim, Sofie Botegård, Axel Steuerer
Copenhagen: Kim Lefmann, Linda Udby, Anette Vickery, Kaspar Hewitt Klenø, Mads Bertelsen, Morten Sales, Carsten Cooper-Jensen, Heloisa Nunes Bordallo
Risø-DTU: Peter Kjær Willendrup, Britt Rosendahl Hansen
HZB: Klaus Lieutenant
ILL: (observer: Emmanuel Farhi)

(Excused: Carina Höglund, Uwe Filges, Sonja Lindahl Holm, Lars von Moos, Esben Klinkby, Pascale Deen, Johan Jacobsen, Jonas Okkels Birk, Mogens Christensen (obs.), Niels Bech Christensen (obs.))

Agenda

0. Instrumentation: Powder diffractometers
1. Science: Structure of hydrogen materials
2. News related to ESS
3. Reports
 1. New ideas for guide materials
 2. Long guide transmissions
4. The ToDo list
5. Priorities and distribution of future tasks
6. Future meetings
7. Any Other Business

Minutes also contains

Updated ToDo and priority list for the Simulation Group

0. Instrumentation: Powder diffraction

Paul Henry presented a powder diffraction tutorial, including his ideas for powder diffraction at the ESS. The full presentation will be present at the home page www.esss.dk . Below is presented selected main points of the presentation.

The developments in the last 10-15 years has been towards time-resolved studies, in particular in-situ studies of chemical reactions. The need is sufficient flux, resolution, and signal-to-noise ratio. In addition, the proper (complex) sample environment should be present, and the neutron data should ideally be taken simultaneous with other measurement techniques (e.g. UV, Raman, TGA, X-ray, ...?). Software to analyze the huge amount of data is urgently needed.

1. Science: Hydrogen-containing materials

PH presented the his own research in hydrogen-containing materials. Of particular interest to simulators was the information that the hydrogen incoherent scattering cross section varies with wavelength. This information must be incorporated into the packages.

The full presentation will be present at the home page www.esss.dk .

Action items:

- Place PH presentations on the home page (BRH)
- Incorporate hydrogen incoherent scattering into McStas and VITESS (Kle, PKW, and KLi)

2. News related to ESS

KHA presented the latest news from ESS:

- UK is now a member of the ESS consortium, after CCLRC agreed to support Lund as a site and work for the realization of ESS. UK financial contributions are still unclear. ISIS staff is eager to contribute.
- New employments etc.:
 - Oliver Kirstein, leader of neutron instrument techniques groups, from 15 May
 - Arno Hiess, leader of ESS science program, from 1 June (75% at ESS)
 - Pascale Deen, presently on maternity leave; back around October
- We repeated the list of “personal simulators”
 - Chopper spectrometers: AV, KHK
 - Reflectometry: AV (KLi)
 - Imaging: (KLi)
 - Powder diffraction: HJ (KLe)
 - SANS: KHK
 - Protein + single crystal diffractometers: BRH
 - Single crystal spectrometer: JOB (Kle)
- The timeline for the design update phase – as for the full ESS - is unchanged. Therefore, we MUST be ready with the technical design report (TDR) in December 2012. In the TDR, we need presentations of 7 instruments. These are not the same at the selected 7 instruments for

day-1, but there is likely to be an overlap. It is our responsibility that these instruments are well described and simulated! The 7 instruments are mostly bi-spectral:

- Cold Chopper Spectrometer
 - Narrow Bandwidth thermal powder diffractometer
 - Small-sample (bio-) SANS
 - Horizontal (bio-) reflectometer
 - Protein Crystallography diffractometer
 - High-resolution imaging station
 - Crystal analyzer spectrometer (TOFTAS)
- When the TDR has been submitted, there will be a funding gap, while the countries sign up for participation. The Swedish government will fill this gap meanwhile. We hope this will happen in Denmark as well!
 - ESS proposes a new time structure: 2.85 ms pulse length and 14 Hz (72 ms), giving 1/25 duty cycle and 5 MW at 50 mA accelerator current. DK group must answer if we can simulate the FoM for this time structure before the SAC meeting late May.

Action Items:

- Kle answer to KHA if we can simulate new time structure before late May.

3. Projects:

3.1 New ideas for guide materials

CCJ presented his ideas for new concepts for materials for guide coating and shielding materials. The basic idea is that neutrons rejected by the guide system should cause as little background as possible; both to improve measured data and to reduce the cost of shielding.

For guide coating material, Be and diamond-like carbon was suggested, while Ni-58 / Ni-62 was rejected due to high price of Ni-62. For shielding materials, it was suggested to abandon B and aim for materials with smaller gamma energies (although the total gamma dose may be higher).

This presentation spawned a lengthy discussion.

The full presentation will be present at the home page www.esss.dk .

3.2 Long guide comparison

KHK presented the update of the VITESS-McStas guide simulation project. The general trend is that long guides, up to 150 m, transport neutrons extremely well. The Liouville efficiency is usually 80-90%; and 50% for the difficult case with thermal neutrons with large (2 degrees) divergences. VITESS and McStas agree with small discrepancies, and elliptical and parabolic-straight-parabolic guides have similar performance, with the elliptical being slightly better.

This work, including transport of brilliance in long guides vs. shape and waviness, should be presented to the SAC meeting in late May. It would be preferable if a short report would be written up before May 2. We must find out if we have time to do 300 m guide before the SAC meeting.

CCJ presented the idea that at long instruments the 300 m guides could be replaced by KB-type mirrors, reflecting only around one certain q-value.

The full presentation will be present at the home page www.esss.dk .

Action items:

- Place KHK+CCJ presentations on home page (BRH)
- Make short write-up of guide simulations to SAC (KHK, KLi, Kle)
- Determine if 300 m simulation can be done for the May SAC (KHK, KLi)
- Iron out last discrepancies between McStas and VITESS on guides (KHK, KLi)

4. Minutes and the ToDo list

4.1 Approving minutes from March 2011

The minutes have been discussed by Kle and KHA and at the Danish group meetings; and have in general been present at the repository. Comments have been incorporated into the final version.

4.2 ToDo list of the ESS simulation group

The ToDo list from the March 2011 minutes was traversed.

- A number of items on the list were finalized since last meeting and were deleted.
- Items not found of sufficient priority were deleted to shorten the list.
- Not all priority items were done, in particular the ones concerned with writing articles and reports.
- Remaining ToDo items are listed at the last pages of these minutes.

5. Priorities and distributions of tasks

We here identified the need of simulating beam extraction systems, i.e. Eye-of-the needle geometries, bispectral extraction systems, and a combination of those.

The new bispectral source is supposedly a 12x12 cm² cold source, embedded in a 24x24 cm² thermal source. The comparison between normal and bispectral should be made for 0.1, 0.5, and 2.0 degrees divergence, the a 1x1 cm² sample, and 150 m guides. We keep 16 2/3 Hz and 2 ms and use wavelength bands centered at 1.5 Å, 3.0 Å and 5.0Å. KLi and Kle writes a document about this.

From the tasks on the ToDo list, the following items were selected as priorities (some unchanged from the February meeting):

1. Finalize the simulations of protein crystallography station (BRH)
Submit paper on the time structure comparisons (Kle and KHA)
Update one-pagers on the time structure simulations (all)
Simulate 7 Flagship Instruments:
 - Angular-dispersive powder diffractometer (HJ)
 - Horizontal reflectometer (coordinate with German group) (AV, Kle)
 - Imaging station (done by German groups) (KLi)
 - Cold Chopper (mostly OK) (Kle, KHK)
 - TOFTAS (doing well) (JOB, JJ)
 - Protein crystallography (BRH)

Small-sample SANS (KHK)

! Simulate beam extraction systems ! (JJ, SLH, KHK, KLe)

2. Finish Ven paper (Kle, AV, KHA)

Write the reports on selected instrument simulations (all)

Finalize last items on guide comparisons; write up (KHK and KLi)

6. Future meetings

Meetings of this group will in general be held second Wednesday of each month, alternating between Lund and Copenhagen. However, next meeting is placed differently:

- 1st June in Copenhagen: Thermal spectrometer comparison (AV) + Science talk (AH)

In addition, there is a topical meeting on guide extraction systems (?? before or after)

The HZB group is growing, and the Prague group has taken interest in this activity. All members from HZB and Prague (and all other ESS teams from anywhere) are welcome at these monthly meetings.

7. AoB

(none)

Updated ToDo list for the Simulation Group, 24/4-11

From November 2010:

- We should in general write papers on what is significant, for now, this includes
 - Ven meeting (KLi writes about SANS. KLe will finish thermal spectrometer)
 - Time structure (first priority, KHA to write a conclusion section on accelerator parameters, Kle to finalize and submit. One-pagers as URL)
 - Guides (KHK, Kle, KLi, and KHA; for ECNS proceedings)

From December 2010:

- Finish the instrument model, protein crystallography (BRH)
- UF: run MCNPX simulations on background for short instruments

From January 2011:

- PJ and MB continue the simulations to investigate other moderator shapes, e.g. sawtooth, and to include beam divergence; include realistic reflector behaviour; incorporate into McStas.
- PJ and MB will build a “Farnworth fuser” neutron source with moderator for test purposes.
- PKW, KHA, KLi, HNB (+EF): continue the work on source descriptions to reach a common description in both packages; collect data from other sources (HZB, FRM-2, PSI, ...); put source data on repository.
- Kle: Discuss ECNS satellite proceeding issues with Journal of Neutron Research

From February 2011:

- Investigate half-ellipse + straight + half-ellipse guide shape (KHK)
- Reproduce the VITESS transmittance vs. waviness curve with McStas (KHK, KLi)

From March 2011:

- Place PD, EF and KLi presentations on home page (BRH)
- Investigate how optimizers tolerate noise (EF)

From April 2011:

- Kle answer to KHA if we can simulate new time structure before late May.
- Place PH+KHK+CCJ presentations on home page (BRH)
- Iron out last discrepancies between McStas and VITESS on guides (KHK, KLi)
- Make short write-up of guide waviness etc. to SAC (KHK, KLi, Kle)

- Determine if 300 m guide simulation can be done for the SAC (KHK, KLi)
- Incorporate hydrogen incoherent scattering into McStas and VITESS (Kle, PKW, and KLi)
- Define a list of instruments, where we should write a report (including authors): “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. The reports will all be written in LaTeX and will follow the outline given by the Reflectometer example.” (KLe)
- Make beam extraction studies
 - Write a simulation definition document (Kle and KLi)
 - Comparison of settings with bispectral mirror and 6m eye-of-the-needle: (normal, eye-of-the-needle, bispectral, both) x (thermal, cold) x (0.5, 2 deg div.) (JJ, SLH, KLi, KLe)
 - Make prototype of guide long-eye-of-the-needle; test with cold diffractometer (SLH)
 - Find geometry of J-PARC eye-of-the-needle construction

From SAC meeting, November 2010:

- Estimate instrument gain factors over J-PARC, SNS, ISIS, ILL
 - Compare protein diffractometers with LMX at ISIS
 - Compare thermal 180 m powder machine with GEM
 - Compare long SANS with existing instruments (D22?)
 - Compare backscatter spectrometer to BASIS at SNS (at same resolution)
 - Compare TOFTAS to TAS at ESS and at ILL
- Simulate different thermal powder diffractometers + thermal spectrometer designs
- Simulate combination of SANS and cold powder machine