Minutes from Simulator's meeting

Copenhagen, November 30, 2011

0) presentation of the 25 participants:

**NBI:** Jonas Okkels Birk, Johannels Beil, Sonja Holm, Anette Vickery, Linda Udby, Kaspar Klenø, Johan Jacobsen, Kim Lefmann

**DTU:** Britt R. Hansen, Esben Klinkby, Peter Willendrup

**AU Århus:** Mogens Christensen

**TUM-FRM II:** Giovanna Simeoni, Luca Silvi

**ESS:** Paul Henry, Andrew Jackson, Oliver Kirstein, Markus Strobl, Hanna Wacklin, Ken Andersen

**HZG:** Mustapha Rouijaa, Jochen Fenske

**HZB:** Klaus Lieutenant

**NPI Rez:** Jan Saroun

**PSI:** Uwe Filges

1. News from ESS: (Ken)

Andrew Jackson, instrument scientist for Small Angle Scattering has arrived. Another instrument scientist for spectrocopy will soon be employed, - ESS has recently held interviews for the position. The spectroscopy instrument scientist will be the 7th instrument scientist employed at ESS.

News from SAC: (Ken)

3 items:

I) *regarding the time structure base line change:* it is clear that the time structure has a large impact on the different instrument designs. The change from 20Hz to 14Hz was endorsed by the SAC, but is not yet official, as it needs a decision of the Steering Committee. We should continue working with this structure.

II) *regarding the instrument program plan:* a document which describes how the different WP are managed in an as coherent way as possible is produced, this document also includes a timeline for choosing instruments.

III) *regarding the instrument selection process:* a series of workshops (in september 2012) aiming at choosing the instruments together with the user community has been proposed. However, the SAC saw this as an invitation to the users to 'voting' about the different instruments, so the idea about the workshops was not supported the SAC. They would rather see ESS take the leadership and decide. The user community will be involved in the decisions through the IKON workshops and Science and Scientist meetings, where users are invited to present their ideas.

So, in conclusion: there will be a cancellation of the September workshops.

Currently there are active discussions taking place between ESS and with Czech and Dutch labs, so Ken expect that rather quickly their WP's will also be integrated into ESS.

There has been a workshop with MAX4 and universities about education in X-ray and Neutron science. The workshop gave a positive impact on the planning of the scientific infrastructure between ESS and MAX4, including guesthouse, deuteration facilities and much more.

Kim Lefmann asked Ken if he could confirm a rumor that was presented to him: has a decision been made that there will be only a bispectral source and no cold source? This rumor cannot be confirmed by Ken, at present the plan is to have both a thermal and cold moderator, keeping the possibilities of having bispectral, cold, thermal sources.

1. News from groups:

Kim: explaining the role of the Copenhagen group. Everyone in the group stated their areas of interest and who they are working with:

Anette: TAS, Thermal Chopper (Pascale Deen, ESS), Reflectometry (Hanna Wacklin, ESS)

Sonja: narrow bandwidth powder (Paul Henry, ESS)

Johannes: simulation reflectometry (Jochen Stahn, PSI)

Jonas: inverse TOF flatcone

Johan: simulation of the TOF flatcone together with Jonas, and backscattering

Peter: McStas debugging and development, supporting Britt's simulations, working with Esben towards target station development

Esben: interfacing McStas with MCNPX

Kaspar: guide optics, design (Pascale Deen, ESS)

Linda: virtual and real experiments, teaching methods. Not directly related to ESS

Britt: simulation of Macromolecular diffraction, working with (Esko Oksanen, ESS)

TUM: Current work is focused on TOF spectroscopy and chopper development. Both Multispectral, broadband spectrometers and high resolution spectrometers are investigated.

PSI: Current work is focused on chopper instruments, small angle scattering, reflectometer and optics WP. The WP starts in January 2012, so they are looking for post docs to be involved in instrument control, moderator design and couple MCNPX and McStas, working with Peter and Esben from the Copenhagen group. Also filter systems for fast neutrons will be investigated.

Ken commented that there is not yet any formal contract between ESS and any of the various in-kind contributions on instruments.

NPI: TOF instruments are simulated with Restrax. 2 concepts for a diffractometer have been simulated, one with crystal mono and another with TOF. They have worked with a detailed optimization of slit systems and optics. Investigation of how instruments at existing sources will perform at the ESS source.

Peter Willendrup: announced that there has been a reorganisation of the Risø/DTU group: Britt and Peter is moving to physics at DTU together with the scattering people. Esben is staying at Risø.

Berlin: HZB is involved in many WP's. Main activity is development of Vitess. Klaus mentioned a general purpose diffractometer, spectrometer, alternative methods involving spin echo ideas.

1 post doc working on each of the three instruments, helping on progress on the Vitess package.

HZG: progress in diffraction, new colleague just started. The instrument simulations are just getting started, until now they have performed numerical calculations.

Half an hour break to make space for individual discussion among people....

1. Science talk from ESS:

Andrew Jackson, Instrument Scientist, ESS : Small Angle Scattering

Half an hour break to make space for individual discussion among people....

1. Simulation presentations:

Kaspar Klenø: recap and update on guide simulations. Comment from Klaus: there is no simple relationship between sample size and guide width

Kim: Simulation of TOF resolution . If anyone like to have the McStas components needed for this, Kim will provide them a copy.

The calculation of errorbars: postponed till later

1. Status on articles and conferences:

**ICANS: March 4-9 2012**

List of people sending in abstracts (marked with \* are sure that they are going):

\*Klaus Lieutenant

\*Peter Willendrup

\*Esben Klinkby

\*Pascale Deen

\*Ken Andersen

Paul Henry

Markus Strobl

Hanna Wacklin

Klaus Habicht: related to general activities on HZB

Jörg Voigt

In addition, the Copenhagen group will send in abstracts on TOFTAS (Johan, Jonas) and Guides simulations (Kaspar).

**IKON2: February 9-10 2012, Malmø:**

parallel sessions on each WP. At least 1 person should be present from each WP to represent simulation work.

**Science and Scientist: April 19-20 2012, Berlin:**

Bring as many future users together as possible. There will 6-7 parallel sessions, Ken would like to have at least 1 in each session to represent simulation work.

**New call for Science Symposia** will be out soon, deadline will be at the end of January 2012, the meeting will be taking place 2nd half of 2012.

**Status on articles:**

Kim pointed out that it is important to publish simulation work. Relevant journals could be

*i) Journal of Neutron Research, ii) NIMA*

The affiliation for the ones working with ESS should be

ESS Design Update Programme – COUNTRY + the University affiliation.

Time Structure simulations: Paper almost ready to be published. Kim to discuss a few things with Ken.

1. AoB:

Klaus Lieutenant: Suggestion of replacing some, but not all of the meetings with a video conference. People from e.g. Germany are spending a lot of time and money to go Copenhagen/Lund. There is no suitable room at KU or at ESS, but there exist a video room at DTU. Peter Willendrup has a solution which will be useful for the next meetings.

Hanna suggests small meetings on Skype on topics on the agenda before the meeting.

It was suggested to have satellite meetings before and after the ICON meetings.

News from Swiss Neutronics: Kim, Kaspar, Carsten Cooper-Jensen and Ursula Hansen went to Swiss-Neutronics. The size of the mirrors and other parameters used in simulations was confirmed by Swiss Neutronics to be realistic. The capacity for guide construction may not exist with the current facilities, unless guide manufacturers increase their capacity.

ESS is aware of this issue, and are considering solutions.

It was decided that future simulation meetings should be centred around a particular theme. The relevant instrument scientist(s) should invite external people to participate as appropriate. NEXT meetings (with theme):

18/1/12 in Lund: Spectroscopy (choppers, TOFTAS, backscattering)

29/2/12 in Copenhagen: Reflectometry

28/3/12 in Lund: S&S Meeting in Berlin

9/5/12 in Copenhagen: diffraction (both powder and protein)

6/6/12 in Lund: theme to be defined

4/7/12 in Copenhagen: theme to be defined