* Present: Esko Oksanen, Johan Jacobson, Sonja Lindahl Holm, Paul Henry, Kaspar Klenø, Kim Lefman, Esben Bryndt Klinkby, Konstantin Balashev, Anette, Linda Udby, Peter Willendrup, Heloisa Bordallo, Marcus Strobl, Ken Andersen, Ruep Lechner.
* Agenda:
* 1. News from ESS and German meetings - Ken
* 2. Science talk – Esko Oksanen
* 3. Simulation proceedings
* - Kaspar: guide comparison, part III
* - Anette: comparing thermal spectrometers, virtual experiments, part I
* - Kim: Beam extraction, part I
* 4. Collaboration between simulators and target
* 5. Organisation, manpower, priorities
* 6. AoB
* 7. Actions
* 1. News from ESS and German meetings – Ken Andersen
* **New Staff:** new instrument scientists at ESS

- Marcus Strobl (Imaging)

- Esko Oksanen (Macromolecular Crystallography)

- Andrew Jackson (SANS) to arrive last week of November.

- a position for spectroscopy is currently advertised

* **Recent meetings:**
* - first IKON conference in Lund 8th of September with satellite workpackage
* - workshop on a hybrid SANS-Imaging-Powder Diffractomet in Sønderborg
* - organized by the Swiss-Danish workpackage 4(M.Cristensen).
* - JCNS in Tutzing 4-7 October
* - ESS Science meeting for German KFN users in Bad Reichenhall 10-12 October.
* - An ESS Instruments day 25th of October was held to obtain an overview of the current status and outlook of all instrument projects. While we are well on track for submission of the TDR, it was agreed that the instrument selection process is the real milestone – this will happened at annual user workshops for ~3 instruments per year to select the instrument projects for construction based on their merit and maturity.
* On the in simulation front, meetings between instrument scientists and dedicated simulators on a twice monthly basis will now go ahead in order to keep work on track. In the in kind workpackages there has been a certain need to weed out some unnecessary repetition in different instrument workpackages, with some reorientation/rationalization of the work to maximize output. Marcus Strobl pointed out that it may sometimes be good however if two groups work on same thing for more overall confidence in the results, but that this requires good communication.
* At ESS the instrument group uses a Plone document handling system temporarily and it was discussed how the DMSC would get access and share the documentation. It was agree that while not everyone needs to have a Plone account, it should be able to upload material relevant to the workpackages there and to have a link to the esss.dk homepage from Plone. Konstantin. ACTION FOR KEN: send mail to Konstantin about which access rights to give to the simulation group members and mail DMSC a link to the Plone registration page.
* **Conceptual Design Report:** The 1st draft of the CDR was submitted in September including a draft preliminary instrument suite, science cases etc. This is an ESS internal document for the STC – but it was agreed that the final version submitted in November 2011 would be useful for DMSC members.
* 2. Science talk - Esko Oksanen: Suprising protonation states of Urate oxidase

Esko decribed the challenges involved in a neutron protein diffraction experiment, from the process of growing mm-size crystal to solving the structures and fitting 10 000s to millions of reflections. The question was asked whether there are prospects for proteins studies by powder diffraction – this is usually impossible to resolve due to the very large unit cell size (up to 300Å) – also because high quality structure factor with less than 0.5% errors are needed for direct structure determination.

* Kim Lefman posed a question on the highly specialised data-analysis – what are the needs for development at ESS?
* A: TOF Laue patterns are challenging and needs software development to extract intensities from images, but the rest of the analysis is very similar to X-rays for which the main analysis packaged is the Phoenix program developed at Lawrence Livermore National Laboratory (the developers are open to include joint refinement with neutrons, including QM models). As such there is no need for ESS specific refinement tools.
* Ken Andersen wondered what will be the future demand from X-ray crystallography community to see the hygrogens?
* A: This will be very important, but most X-ray crystallography users today don’t know that neutrons exist, or think that they only work with lysozyme! In the best case both techniques would use the same physical crystal but in reality the crystals for X-rays (50 μm) are too small for neutron work. The limit is the number of unit cells needed to a crystal structure is ~20, which implies that we should be able to use microcrystals for small molecule diffraction instead of cm2.
* Kim Lefman asked about the specific instrument requirements - these include high flux, low background and resolution of diffraction spots on detector for unit cell size up to 300Å – ideally an instrument would have a movable detector distance and a suitable divergence of the order of the crystal mosaicity.
* Ken Andersen commented that macromolecular crystallography is one of the techniques predicted to do very well at ESS and to be able to use the full flux gain (factor of 30 to LADI), and also benefit from the dissipation of background in time-of-flight. Wavelengths suitable would be 1.5-3.5Å approx. indicating a bispectral set upt - 150m vs 75m instruments are considered.
* 3. Simulation proceedings.
* **Kaspar Klenø: guide comparison, part III – update IV.**
* Kaspar presented the brilliance transfer of thermal neutrons in 150m M=3 guides with 2 deg divergence, wavelength band 0.75-2.25Å weighted by the Maxwellian distribution of the H2O moderator. M=3 coating. There is a minimum at 0.5 deg divergence for the ballistic guide shape which comes from the focusing section, whereas the parabolic guide has a dip at 0.25deg. An elliptical guide with a straight section in the middle is useless for thermal neutrons (although ss useless for cold). An Elliptical-straight-parabolic hybrid guide (M=6, M=3 which could contribute to dip) has a smaller dip but loses divergence above 1.4 deg. However the current optimization was done for geometry vs integrated flux – there is more flux at high div, hence this dominates the results and for optimization for lower divergence a different figure of merit should be used. The question was raised how many applications will want 2deg divergence – it seems that the 0.5 divergence parabolic guide would very good for < 1ded divergence. Coating optimization will be the next step of the study, from which a complete report will soon be complied, a preliminary report already available.
* **Anette: comparing thermal spectrometers, virtual experiments, part I**
* Anette presented the project which was started 3 years ago by Klaus Habicht at HZB - using TAS with a straight guide and 1:1 doubly focusing monochromator . Currrent work has been to complete the simulations of the primary spectrometer using as a figure of merit (flux2/energy spread). An elliptical guide, doubly non-equidistant focusing monochromator. Was optimized. Accepting an increased divergence (with similar energy resolution) has been used to gain in flux an order of magnitude compared to earlier simulations. Virtual experiments with a magnon with 2meV gap were used to test the instrument. Conclusion – makeover of TAS a success. Outlook – virtual experiment with thermal neutrons and optimization for 25meV energies and a 300m guide should be done. Comparison to a thermal chopper spectrometer will follow.
* Ken Andersen suggested that a TOF-TAS instrument should also eventually be included in a three-way comparison (Johan Jacobnsen has already has done the TAS end).
* Kim Lefman mentioned an IN4 type instrument (from the Ven) meeting, which could perhaps be used but it would need a lot more work. A Crystal monochromator chopper spectrometer is not covered at present.
* **Kim Lefman : Beam extraction, part I**
* Kim presented the status of ongoing work on the beam extraction. Considered extraction systems included:
* A) Termal-elliptical, focusing guide
* B) Cold elliptical guide
* C) Thermal/cold-elliptical guide
* D) Pinhole-elliptical buide - (results indicate that a 1cm source pin hole needs 3cm sample – this is due to the coma aberration)
* E) Eye-of-the-needle beamsplit with virtual source after elliptical guide to select part of divergence (split it in several beams) – 35% thermal neutrons 1cm2 but not on optical axis. Only started this week.
* For the bispectral geometry with a curved doubly focusing mirror the figure of merit (thermal flux 0.75-2.25Å) + cold flux (4.25 – 5.75Å) was used. It looks like this leads to solutions with loss of intensity (30%) in exactly the gap region region! The guides start directly from the mirror but were compared to standard thermal/cold (optimized respectively) guides that start from much closer to the source and this might lead to an overestimation of the losses.
* Kaspar suggested to normalize against the intensity for each wavelength bin as a better figure of merit.
* The question was asked of the moderator liaisons (Konstantin/Esben), what the angular and height distribution of the moderator emittance will look like?
* Kim’s conclusion was that the bispectral moderator couples reasonably well to an elliptical guide with relatively mall losses (~20%) and only slight problems in cross over region. McStas/VITESS were shown to be in good agreement. Ken Andersen considered this great news although there is still a lot to optimize (guides above/below) – the wavelength ranges should be adapted for the figure of merit to judge the losses properly. There is room for input for further work.
* Sonja has been working on a guide-splitting model using straight guides for short sections after the main elliptical guide. This would allow splitting the full flux for instruments that do not need large divergence and would be cheaper to have several instruments feeding off same guide than to build them separately, especially for long guides. However this is only possible if the instruments can use the same choppers/resolution/bandwidth.
* Beam splitting is not just limited to long guides and it could be used to effectively multiply instruments – e.g. crystal monochoromator instruments, protein diffractomers, (SANS)? ACTION – INVESTIGATE INSTRUMENT FARMS & SEND RESULTS TO SONJA FOR SIMULATION.
* Ken Andersen initiated a discussion on the position of pulse shaping choppers & bispectral extraction, which might mean no longer being in the optimal position for pulse shaping. The beam should focus into the chopper position at 6m as much as possible in order to have a small beam and small choppers there. The Size/speed restrictions on choppers at 6m (70cm diameter for 5deg) should be designed with view to reliability and little need for maintenance – they should not be running at th edge of their capavity.
* Kaspar asked for a definition of a small beam for this purpose? ACTION What is this (1,2,3-4cm or…) – quantify this for getting e.g. 80% of flux on sample and send to him.
* Ruep Lechner pointed out that different optimizations for instruments that can use wide divergence on very small samples would be necessary but this can be achieved by focusing elements at the end of guide. Would it be possible to include something like this in McStas? Maybe this could be done only in 2D to same computing power, since directions completely decoupled. Sonja & Henrik Jacobsen.
* 4. Collaboration between simulators and target
* ACTION – put together list of desirable and critical target parameters (brightness etc.) in smaller meeting & give to target in the frame work of beam extraction meetings.
* Who is working on moderator calculations in DK? Esben, Mads Bertelsen (simple, fast models of geometries (grooves)) are working on moderator calculations now, with the source code implemented in McStas from 2001 calculations – is there something more recent? No, and should look at old McStas code when starting to provide new code to save time.
* 5. Organisation, manpower, priorities
* Ken: the priority is now on spending time with instrument scientists working on instruments. Look for possibilities to combine some guide optimisations with specific instruments to make sure they will be ready for the instrument selection process. Kim expressed a wish to still keep some simulations general for later use.

**DK WP work: First priority**

* Multi-beam reflectometry: Anette Vickery (50-50 with thermal chopper, then as the main person from January), Johannes Beil as the main person at the moment
* Thermal chopper: Kim, Anette until January, Henrik from January
* Narrow-BW powder: Sonja – 80% of her time. Will be available in few weeks.
* Macromolecular crystallography: Britt Rosendahl Hansen, as her main task
* Backscattering: Heloisa & Ruep, Johan from about January

**DK-CH WPs: Second priority**

* small-sample SANS
* crystal-analyser: Johan Jacobsen until January, then Jonas
* Selene: off-specular reflectivity and gravity (Peter W)
* Hybrid diff-SANS-imaging

**Cross-instrument tasks: Also first priority**

* Beam extraction incl. bispectral: Klaus L, Henrik Jacobsen until January, Kaspar from January. Various instruments will feed their specifications into this task. Two separate tasks: Eye of the needle and bispectral switch. Kim will contact Klaus to arrange sharing between CPH and HZB.
* Long guides: finish off this task with paper by Kaspar, then move simulations into specific instruments.
* Guide split: Sonja will give advice to Britt for protein diffractometer. Task to be picked up at a later stage.

**Other tasks:**

* Esben: occupied with WP2.? for Target on MCNP-McStas integration and Beam Extraction for Target.
* Peter W: overall responsibility for source brightness database
* 6. AoB
* **Instrument workshops:** are being rethought for September – to be presented to SAC4.

**Future meetings:**

Once a month, alternating between Cph and Lund, running 10:00-15:00

Standard agenda will be:

1) information on ESS project

2) science presentation

3) presentations on instrument design work

4) AOB

One person from the hosting lab will takes notes of the main actions. The meeting will be followed by a smaller meeting of Ken, Markus, Kim, Peter in which we go through the action list and set priorities for the coming work.

7. ACTIONS:

1. Ken to send mail to Konstantin about which access rights to give to the simulation group members and mail DMSC a link to the Plone registration page.

2. Investigate instrument farms & send results to Sonja for simulation of split guides.

* 3. What is the appropriate extracted beam size (1- 4cm?) – quantify this for getting e.g. 80% of flux on sample and send to Kaspar.
* 4. Compile list of desirable and critical target parameters (brightness etc.) in smaller meeting & give to target in the frame work of beam extraction meetings.