Simulator's meeting at ESS, Lund Oct. 24 2012
Minutes by Anette Vickery/Copenhagen

List of participants:
Anette Vickery
Kim Lefmann
Damian Martin-Rodriguez
Nikolo Violini
Nikolas Tsapatsaris
Marcu Strobl
Britt Rosendahl Hansen
Peter Willendrup
Mogens Christensen
Konstantin Batkov
Klaus Lieutenant
Werner Schweika
Esko Oksanen
Paul Henry
Phil Bentley
Jan Soroun
Pascale Deen

Ken Andersen, Mads Bertelsen, Sonja Holm are ill

List of presentations:
Paul Henry: Powder Monochromatic powder diffraction instrument for ESS.
Nicolo Violini: Bi-spectral powder diffractometer: POW-HOW guide design update
Werner Schweika: POWHOW chopper system.
Klaus Lieutenant: POWHOW: simulations of Guide and Chopper System.
Klaus Lieutenant: Bispectral extraction system
Klaus Lieutenant: Simulations of the Extreme Environment Instrument for the ESS – ESSSEX
Esko Oksanen: Macromolecular Diffractometer at the ESS
Peter Willendrup: Magnetism Diffractometer at ESS
Werner Schweika: Magnetism TOF Laue Diffractometer
Jan Saroun: Complex environment engineering diffractometer

Presentaion by Paul Henry:
Monochromatic powder diffraction instrument for ESS.

In general the simple view from 'outside' is that there is (almost) no flux gain/other advantages compared to an instrument on a short pulsed source, so therefore a monochromatic powder diffraction instrument shouldn't be built at the ESS.

Paul presents a number of advantages of having a monochromatic powder diffraction instrument at the ESS:
Wavelength Frame Multiplication: At relaxed wavelength resolution there is a flux gain compared to short pulsed source instruments. Pascale adds that if one also takes prompt pulse into account (background!), we gain factor ~10.

Monochromatic: The instrument uses full pulse, shorter instrument, flexible resolution/flux trade, chemical crystallography due to limited Qmax.
We can gain a background reduction by using pulsed a source, since we are only counting in a limited time window.

The concept currently being investigated: The current concept is like a pulsed version of D20. It features a primary guide with a feeder. The guide may be half-elliptical or straight. At the current D20 the guide is a 15m flight tube 15m which is not evacuated.
The plan is to investigate the properties of several types of monochromators (germanium, diamond, composite, others...)
The instrument will have a large area detector with TOF resolution and event recording ability.
With the TOF resolution it will be possible to separate lambda/2, lambda/3 at the detector.
That will provide an immediate gain both in Q-range coverage and count rate. The advantage offered by multi wavelength data collection depends on instrument length and developments in available monochromator types.

Detector: Limited access to He3. Investigate other technologies, solid state boron thin films and others.

Separate coherent/incoherent scattering: Paul presents a method to separate coherent/incoherent scattering. It depends on sample-detector distance, sample temperature and incident wavelength. Werner+Kim suggests to use simulations as supplement tool for separating incoherent/coherent. Mads Bertelsen's phd project is focused on development of virtual samples.

Elastic/inenlastic/QENS measurements: Add a pulse shaping chopper

Summary:
simulate and optimise beam transport
compare with existing instruments
one or several instruments on guide
detector development
monochromator development

Timeline: one 2year post doc position, 50% science/50% instrumentation will soon be opened

Presentation by Nicolo Violini:
Bi-spectral powder diffractometer: POW-HOW guide design update

Nicolo sketches the development if the POW-HOW guide concept:
Sep 2011: Eye-of-the-needle + Ellipse
Feb 2012: Eye-of-the-needle + double Ellipse
Apr 2012: systematic performance study of double elliptic guides
They have used a backtracing method to optimize the progressive coating
A beam stop is positioned in the first ellipse

Nicolo compares the simulation results to a reference case: a single elliptic guide optimized by M. Bertelsen, Cph group. He presents simulation data at lambda=1Å, a schematic view of the guides with the coating distribution in color scale.

Results for the double ellipse:
They compare simulated guides with SQUARE and OCTOGONAL cross-sections:
SQUARE: high brilliance transfer, however the homogeneity in position and divergence is spoiled.
OCTOGONAL: high brilliance transfer for 0.4x0.4 cm2 sample size and an improvement of the divergence distribution
Adding a straight central section doesn't increase performance, but it preserves the position and divergence homogeneity.
Increasing the openings to 1.5x1.5 cm2 leads to higher brilliance transfers.
It is possible to tailor (decrease) the divergence by exchanging the guide end mirrors by absorbers.

Future plans:
Development of the extreme environment instrument at HZB
Consider single ellipse vertical and double ellipse horizontal

Kim: suggests that the initial opening could be higher than 1.5cm vertically.
The two ellipses could by kinked relative to each other to avoid line of sight. Mads Bertelsen will present some results on that on the next guide meeting. Uwe Filges is doing shielding calculations for such a guide, showing that the background is more or less gone: fast neutrons background 100/cm^2/s at sample position

Presentation by Werner Schweika:
POWHOW chopper system.

Presenting prototype detector testing. Efficiency 55% at 1Å for B-10 detector. Similar results for prototype from Jülich.

The POW-HOW chopper system features a beat pulse shaping chopper (PSC):
double disk chopper, d=75cm, counter rotating with 6 openings of different size. That offers a flexible resolution.

Werner presents chopper acceptance diagram x-axis=lambda, y-axis=t, so slope=distance
Next, Klaus will present more details on the chopper system.

Presentation by Klaus Lieutenant:

POWHOW: simulations of Guide and Chopper System.

The most complicated component is the beat PSC: it has 6 windows of different size at each disk. The disks are counter rotating and their axes of rotation are parallel but offset vertically.
The simulations indicate that some contamination of the pulses takes place, so the system is not perfect yet. However, the contamination is very low, by several orders of magnitude. The work continues and ideas exist to remove the contamination.

The TOF spectra are well separated on the detector.

Presentation by Klaus Lieutenant:

Bispectral extraction system:

A transparent mirror in front of the thermal moderator lets the short wavelength pass and reflects long wavelengths. The extraction system is made more compact by replacing the long mirror by several short mirrors. It is investigated how the distance from the moderator to the extraction system affects the performance.

M-value required depends on distance to moderator:
distance 3m require m=5,
distance 5m require m=3,

The extraction system closest to the moderator is slightly better:
Klaus explains the reason for this:
When the extraction system is positioned close to the moderator, there is a higher probability of reflection for divergent thermal neutrons. Since the mirror inclination increases with decreasing distance to moderator, there is a higher probability of transmission for divergent cold neutrons: there will be longer paths through mirror with the mirror longer away from the source

Presentation by Klaus Lieutenant:

Simulations of the Extreme Environment Instrument for the ESS – ESSSEX

The instrument is a diffractometer, a spectrometer and a SANS instrument.

General features: 150m length (as a compromise)
Out of line direct of sight

Requirements: short wavelength for diffraction, long wavelength for SANS. Symmetric divergence distribution (especially for diffraction)

Klaus shows a full drawing of the guide system, now also including measures. In addition he shows some of the work which have been done regarding guide performance (for single wavelengths), spatial and divergence distribution.

SANS: currently the collimation is obtained by adding several slits at the guide end

Chopper system: 14Hz choppers, one 70cm at 7m and 200cm (at 19.9m and 79m)
For diffraction: Beat PSC and a 70cm fast chopper (210, 224Hz)
For spectrometry: Beat PSC and a 70cm fast chopper

Guide optimization: the optimized coating (with low m-values) is compared to m=6 all the way. The optimization is good, since there is no noteworthy difference in the performance,

Extraction system: Compact extraction system, efficiency >75%
Divergence up to ~1.5deg fwhm

Currently work is conducted on simulations of the resolution.

Presentation by Esko Oksanen:
Macromolecular Diffractometer at the ESS
The concept is a Quasi Laue TOF diffractometer with a guide of 156m length, m=1 on three sides, m=1.8 for curving. The wavelength band is approximately 1.8Å. A detector with high spatial resolution <0.3mm is required. Esko want to use the extraction system which yields the best flux for the wavelength interval 1.5-3Å.

beam size <1mm^2
divergence +-0.1deg

In principle one can extract 4 beams from the same beam port.

Detectors: Need R&D to reach <0.3mm spatial resolution with reasonable area.
Solid angle coverage can be traded for unit cell size.
Large unit cells will take longer to collect.

Instrument simulations in McStas: need lots of time to get any statistics, and it is difficult to visualize diffraction patterns.

Visualization: Esko shows how they are now able to splitting reflections into time bins

Presentation by Peter Willendrup:
Magnetism Diffractometer at ESS
Collaboration with Arsen Goukassov, LLB
Work initiated 2008 at the Ven workshop.
Single crystal magnetic experiment
White beam (Laue) Neutron Diffraction from a single crystal.
Length ~40m
Post Doc to be hired at LLB to work on this project.

Presentation by Werner Schweika:
Magnetism TOF Laue Diffractometer
~150m length
thermal+polarization and field: site susceptibilities, spin densities
cold+polarization analysis: magnetic structure determination, diffuse magnetic scattering

There are considerations on using the Selene concept for the 150m guide.

Werner explains the acceptance diagrams used for the chopper positioning, a nice paper by Ken Andersen exist...

Presentation by Jan Saroun

Complex environment engineering diffractometer

Jan presents an updated neutron guide geometry for the diffractometer.
Two new virtual samples for engineering materials have been developed: duplex steel and TiAl alloy.

Jan presents a schematic view of the instrument. Length ~150m ballistic guide with radial collimators around the sample.

Double chopper system simulations:
Resolution choppers at 6m, frame chopper at 21m.
350mm, 140Hz, openings 54deg and 72deg.
Distance between two chopper disk can be changed to change the resolution
High resolution: 0.2m between choppers
Low resolution: 1m between choppers.

Brilliance transfer: without choppers ~75% 1.5Å-6Å.

deltaT/T ~ constant over wavelength range.

Summary: A detailed model of the CEED instrument concept is available.
Small gauge volume is feasible with radial collimators at ~40cm from sample.
The instrument is characterized by a flat wavelength resolution resolution curve, the resolution is tunable due to the double chopper system.
double frame mode: is possible but not easy to configure, it is hard to avoid cross talk effects etc.
tests with virtual samples: gives a basis for inter-comparison and testing data analysis in the future