

Participants: Martin Moche, Jens Karlsson, Rosaria Gandini, Tobias Karlberg, Changrong Ge

Time and Place: 10 am Thursday 24 Aug 2017, PSF floor 3

§1 Next beamtime meeting is **Thursday 16 November 10 am at PSF floor 3!**

Today's beamtime meeting was announced on Monday 21 Aug that was too tight for many research groups to participate. To avoid this in the future we will now announce next beamtime meeting at the actual meeting. Experienced experimentalists prefer to meet newcomers face-to-face to organize remote beamtime being logistically complex with samples from KI/SU/KTH and the remote experiment itself being run both from KI and SU.

§2 Assign Bessy and Diamond experimentalists

Light source	Beamline	Date	Duration	Start	Experimentalists (potential)
Bessy	BL14-1	2017-09-08	24	09:00	Cancel
Diamond	i03	2017-09-23	24	10:00	Rosaria/Tobias/Changrong (Joseph) - remote
Bessy	BL14-1	2017-10-06	24	09:00	Jens/Martin
Diamond	i04-1	2017-10-09	7	10:00	Geoffrey – likely remote
Bessy	BL14-1	2017-10-19	24	09:00	Jens/Martin
Diamond	i03	2017-10-20	16	17:00	Tobias/Rosaria/Changrong(Sarah, Dirk)(Geoffrey)-remote

People in parenthesis are interested in participating in beamtime, however could not make it to today's beamtime meeting and have to contact the experimentalists to participate in the event. More beamtime listed under "Beamtime schedule" at <http://ki.se/en/mbb/psf-mx>

I should remind Diamond that we do not want beamtime shorter than 16 hours!

§3 PRESTO updates – demo two node interactive runs of XDSAPP and XDSGUI with eiger data

Prepare to run 8 jobs with 4 cpu's per job on two compute nodes having 16 processors each

interactive -N 2 --ntasks-per-node=4 -c 4 -t 1:00:00 -A snic2017-1-199

where interactive command above must match MAXIMUM_NUMBER_OF_JOB and MAXIMUM_NUMBER_OF_PROCESSORS in XDS.INP

➤ XDSAPP - use first container when selecting eiger data - **insu6_1_data_000001.h5**

1. module load XDSAPP # load the XDSGUI module
2. xdsapp # start the software
3. click icon Load and select insu6_1_data_000001.h5
4. In xdsapp GUI add
 - No. of jobs 8
 - No. of cpus 4

➤ XDSGUI - use master file when selecting eiger data - **insu6_1_master.h5**

1. module load XDSGUI # load the XDSGUI module
2. xdsgui # start the software
3. find dataset i.e. insu6_1_master.h5 and press generate_XDS.INP
4. edit XDS.INP by adding
 - MAXIMUM_NUMBER_OF_JOBS=8
 - MAXIMUM_NUMBER_OF_PROCESSORS=4

➤ XDSAPP batch script, see <https://www.nsc.liu.se/support/presto/multi-node-scripts/>

- o In a terminal window execute "sbatch xdsapp.script" where xdsapp.script is:

```
#!/bin/sh
#SBATCH -t 0:30:00
```

```
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=4
#SBATCH -A snic2017-1-199
#SBATCH --mail-type=ALL
module load XDSAPP
xdsapp --cmd \
--dir /proj/xray/users/x_marmo/eiger/presto/demo \
-j 8 \
-c 4 \
-i /proj/xray/users/x_marmo/eiger/2015_11_10/insu6_1_data_000001.h5
```

➤ XDSGUI batch script - XDSGUI cannot be run using sbatch