**Open SESAME & Instruct-ERIC Workshop on Remote X-ray Data Collection from European Synchrotrons at the Weizmann Institute of Science  May 14-18, 2018)**

**DLS:**
Experiments will be carried out on I04 beamline http://www.diamond.ac.uk/Beamlines/Mx/I04.html. This is a tuneable beamline with variable beam size from 5 – 100 μm, has a 25 Hz Pilatus 6M, and is equipped with a Smargon multi-axis goniometer. Remote control by installing locally NoMachine software.

**ESRF:**
Experiments will be carried out on ID29, a tunable microbeam with tunable wavelength (6 - 20 keV) http://www.esrf.eu/id29, using MxCUBE3, remote control via Chrome web-browser.

Current outline, as of Feb 11, 2018. Presentation slots will normally be 45 minutes. Coffee breaks will be introduced.

**Monday, May 14**

| | |
|---|---|
| 10:00-11:00 | Opening. **Joel Sussman**, **Rik Wierenga**, **Ada Yonath**, **Alberto Podjarny** |
| 11:00-12:00 | "Experience with remote data collection at APS", **Osnat Herzberg** |
| 12:00-13:00 | How to do remote data collection at the ESRF beam line (including safety sheet, training, submission of the crystals and their meta data to ISPyB, use of the data processing pipelines) (**Alexander Popov**) |

| | |
|---|---|
| 13:00-14:00 | Lunch |

| | |
|---|---|
| 14:00-16:00 | Student talks |
| 16:00-16:30 | Introduction to the computing facilities (**Orly Dym**) |
| 16:30-17:15 | jsCoFE, a CCP4 Cloud Application for structure solution in distributed computing environment (**Eugene Krissinel**) |
| 17:15-18:00 | Any remaining topics related to the remote data collection session at ESRF (**Alexander Popov**, **Gianluca Santoni**) |

| | |
|---|---|
| 18:00 | dinner on campus |

**Tuesday, May 15**

| | |
|---|---|
| 09:00-10:00 | DIALS presentation: as an introduction to data processing in general and what are the specifics of DIALS? including scaling, merging, data quality indicators, details can then also be discussed in the tutorials (**Nick Devenish**) |
| 10:00-12:00 | Remote data collection **demonstration** using test crystals at the ESRF (**Alexander Popov, Gianluca Santoni** |

| | |
|---|---|
| 12:00-13:00 | Lunch |

| | |
|---|---|
| 13:00-24:00 | Remote data collection at ESRF from student or test crystals following a predefined "priority": **(first group-I, then group-II) (remote data collection room)** (**Alexander Popov and Gianluca Santoni**) |
| 14:00-15:30 | **group-II students (in the computer class room)** <br> Dials tutorial (one hour, using a proteinase K test data set) (1 hour) (**Nick Devenish**) |
| 15:30-17:00 | **group-I students (in the computer class room)** <br> Dials tutorial (one hour, using a proteinase K test data set) (1 hour) (**Nick Devenish**) |

| 18:00 | Dinner on campus |
| --- | --- |
| 19:00-21:00 | jsCoFE tutorial (Eugene Krissinel) |

**Wednesday, May 16**

| 09:00-10:00 | ISPyB-API's and uploading the meta data via a home lab LIMS (Rik Wierenga), IceBear demonstration (Ed Daniel) |
| --- | --- |
| 10:00-12:00 | Evaluation of the ESRF data collection by revisiting the ISPyB session with an emphasis on the optimal use of **the structure determination pipelines** (**Alexander Popov**, **Gianluca Santoni**) |
| 12:00-13:00 | Lunch |
| 13:00-14:00 | Structure improvement / Structure validation / PDB-REDO (Robbie Joosten) |
| 14:00-15:30 | How to do remote data collection at the DLS beam line (including safety sheet, training, submission of the crystals and their meta data to ISPyB, use of the data processing pipelines (**Neil Paterson**) |
| 15:30-17:30 | Tutorial on how to improve and validate a structure (**Robbie Joosten**) |
| 18:00 | Festive Dinner |

**Thursday, May 17**

| 09:00-10:00 | The CRIMS structure determination pipeline (**Josan Marquez**) |
| --- | --- |
| 10:00-12:00 | Remote data collection demonstration at DLS using test crystals. (**Neil Paterson**, **Nick Devenish**) |
| 12:00-13:00 | Lunch |
| 13:00-24:00 | Remote data collection at DLS from student or test crystals following a predefined "priority" (**first group-I, then group-II) (remote data collection room)** (**Neil Paterson**, **Nick Devenish**) |
| 24:00-08:00 | Remote data collection from more crystals at DLS (**Lari Lehtiö and Kristian Koski**) |
| | The group-II, and later the group-I students, can work on data processing and structure improvement, structure validation calculations with help of the expert instructors in the computer class room. |
| 18:00 | Dinner on campus |
| 19:00-21:00 | Students working in the computer class room with help of the instructors |

**Friday, May 18**

| 09:00-10:00 | Current and future plans at MAXIV (**Ana Gonzalez**) |
| --- | --- |
| 10:00-12.00 | Evaluation of the DLS data collection by revisiting the ISPyB session with an emphasis on the optimal use of the **structure determination pipelines** (**Neil Peterson**, **Nick Devenish**) |
| 12:00-13:00 | Lunch |
| 13:00-14:00 | Students working in the computer class room  with help of the instructors |

14:00-15:00    Finalizing the data processing, structure improvement, structure validation activities
15:00-16:00    Closing get-together, providing of the certificates, prize for the best student presentation