

PROGRAM OUTLINE

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 mm, 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.

All remote data collection will be done in the **Data collection room**.

All students will have an opportunity to carry out remote data collection, according to a schedule that will be prepared by Orly Dym and Kristian Koski

All other lectures, tutorials and data processing will be at **The David Lopatie conference centre, Kimmel Hall** (except for Monday May 14 which will be at the **Candiotty Building Lecture Hall**).

Monday, May 14

Hour	Subject
09:00-10:00	Registration
	Chairperson: Joel Sussman
10:00-11:00	Opening. Joel Sussman, Rik Wierenga, Ada Yonath, Alberto Podjarny
11:00-11:45	Experience with remote data collection at APS (Osnat Herzberg)
11:45-12:00	Coffee/tea break
12:00-12:45	Safety declaration to sample description in ISPYB, overall view of ISPYB and MXcuBE3 (Stéphanie Monaco)
12:45-14:00	Lunch
	Chair person: Rik Wierenga
14:00-16:00	Student talks

Hour	Subject
16:00- 16:15	Coffee/tea break
16:15- 16:45	Introduction of the computing facilities and the remote data collection scheduling (Orly Dym)
16:45- 17:15	jsCoFE, a CCP4 Cloud Application for structure solution in distributed computing environment (Eugene Krissinel)
17:15- 18:00	Description of some software tools to help your experiments (EDNA characterisation, helical collects, workflows, mesh & collect, BEST mesh (Alexander Popov))
18:30	Dinner on campus, Venue: The Koffler Accelerator (Pelletron)

Tuesday, May 15

Hour	Subject
	Chair person: Lari Lehtiö
09:00- 09:45	DIALS presentation: an introduction to data processing in general and what are the specifics of DIALS, including scaling, merging, data quality indicators (Nick Devenish)
09:45- 10:00	Coffee/tea break
10:00- 12:00	Demonstration of remote data collection on test crystals at the ID29 beam line, ESRF (Alexander Popov & Stéphanie Monaco)
12:00- 13:00	Lunch
12:00- 15:30	Group-I: Remote data collection at ESRF (Alexander Popov, Stéphanie Monaco, Orly Dym, Lari Lehtiö)
13:00- 15:00	group-II: DIALS tutorial (1hr demonstration, then students practicing) (Nick Devenish)
15:00- 15:30	Coffee/tea break
15:30- 17:30	Group-I: DIALS tutorial (1hr demonstration, then students practicing) (Nick Devenish)
15:30- 17:30	Group-II: Remote data collection at ESRF (Alexander Popov, Stéphanie Monaco, Orly Dym, Lari Lehtiö)
18:00	Dinner on campus, Venue: The David Lopatie Conference Centre
19:15- 21:15	jsCoFE tutorial (Eugene Krissinel and Andrey Lebedev)
17:30- 24:00	Continuation of the remote data collection at ESRF (Alexander Popov, Stéphanie Monaco, Lari Lehtiö and Orly Dym)

Hour	Subject
19:00- 24:00	Coffee/tea, available for the remote data collection activities

Wednesday, May 16

Hour	Subject
Chair person: Orly Dym	
09:00- 09:45	ISPyB-API's and uploading the meta data via a home lab LIMS (Rik Wierenga), IceBear demonstration (Ed Daniel)
09:45- 10:00	Coffee/tea break
10:00- 11:45	Automatic structure determination pipelines at ESRF and evaluation of the ESRF data collection by revisiting the ISPyB session (Alexander Popov & Stéphanie Monaco)
11:45- 12:00	Group photo
12:00- 13:00	Lunch
Chair person: Katja Biterova	
13:00- 13:45	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))
13:45- 14:30	Structure improvement / Structure validation / PDB-REDO (Robbie Joosten)
14:30- 14:45	Coffee/tea break
14:45- 17:30	Tutorial on how to improve and validate a structure (1hr demonstration, then students practicing) (Robbie Joosten)
18:00	Leave by busses for Festive Dinner – in Tel Aviv/Jaffa

Thursday, May 17

Hour	Subject
Chair person: Joel Sussman	
09:00- 09:45	The CRIMS structure determination pipeline (Josan Marquez)
09:45- 10:00	Coffee/tea break
10:00- 12:00	Remote data collection demonstration at DLS using test crystals (Neil Paterson & Nick Devenish)

Hour	Subject
12:00-13:00	Lunch
12:00-17:30	Remote data collection at DLS (Neil Paterson, Nick Devenish, Lari Lehtiö & Orly Dym)
15:00-15:30	Coffee/tea break
15:30-17:30	Remote data collection at DLS (Neil Paterson, Nick Devenish, Lari Lehtiö & Orly Dym)
13:00-17:30	Students not involved in remote data collection can work on data processing and structure improvement validation calculations with help of the expert instructors
18:00	Dinner on campus, Venue: The David Lopatie Conference Centre
17:30-24:00	Remote data collection at DLS (Neil Paterson, Nick Devenish, Lari Lehtiö & Orly Dym)
19:15-21:15	Students not involved in remote data collection can work on data processing and structure improvement validation calculations with help of the expert instructors
19:00-24:00	Coffee/tea, available also for the remote data collection activities
24:00-08:00	Oulu remote data collection at DLS (Gabriele Cordara and Kristian Koski)

Friday, May 18

Hour	Subject
09:00-11:00	Finalising the remote data collection at DLS (Neil Paterson, Orly Dym, Lari Lehtiö)
09:00-10:30	Students not involved in remote data collection can evaluate the data collected at DLS by revisiting the ISPyB session with an emphasis on the optimal use of the structure determination pipelines (Nick Devenish)
10:30-11:00	Coffee/tea break
11:00-12:15	Evaluation of the DLS data collection by revisiting the ISPyB session with an emphasis on the optimal use of the structure determination pipelines (Neil Paterson & Nick Devenish)
12:15-12:45	Light Lunch
	Chair person: Joel Sussman
12:45-13:30	Current and future plans at MAX IV (Ana Gonzalez)
13:30-14:00	Integrated approaches for in-house protein crystallography studies (Vernon Smith)

Hour	Subject
14:00-15:00	Closing get-together with snacks and drinks, providing of the certificates, prize for the best student presentation

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