# Serial Crystallography Methods Workshop



Monday, July 17, 2023 - Friday, July 21, 2023

# **Scientific Program**

### Monday July 17th

Welcome Session: Opening session where we say who is who and why are we here Where are we, where are we going? Tell me one thing which is cool, one thing which is a big problem for you?

#### Morning Session (joint):

Aligning experiment methods with data handling and data analysis? Implications for hardware of software requirements, implication for software on hardware requirements.

Afternoon Session:

Lightning introductory talks then split into parallel sessions (joint)

Handling data from "mighty" serial crystallography experiments: generating, processing, storing, archiving - processing energy efficiently also (parallel)

Portability of hardware to other facilities (parallel)

**Tuesday July 18th** Morning Session:

Lightning introductory talks (joint)

Sample delivery / sample handling / remote operation? (parallel)

Software / getting into the weeds on what we need to do - e.g. partiality problem, reflection profile, mosaicity, etc. (parallel)

#### Afternoon Session: (joint)

Developer wrap up - horizon view - what should we be looking for? What should we be doing so that you can use the data you have collected (e.g. using the complementary information, have sufficient data for refinement, etc.)

#### Wednesday July 19th

Morning: Session 1: How can we handle the transition of users from routine to SFX/SSX? Session 2: Recognizing the differences in XFEL and SR SSX (important for users)

Discussion Structure: Intro talk (from moderator) 4 x 5 minute lightning talks Discussion - [panel / open] -with moderator Breakout for coffee, write report Report back at the end of break-out with the conclusion of breakout Afternoon:

Session 1: Synthesizing data for deposition (serial MX, multimodal data sets, etc) Session 2: What's missing in data integration and scaling?

Discussion Structure: Intro talk (from moderator) 4 x 5 minute lightning talks Discussion - [panel / open] -with moderator Breakout for coffee, write report Report back at the end of break-out with the conclusion of breakout

#### Thursday July 20th

*Morning:* Session 1: What are we missing in terms of sample delivery / analysis methods? Session 2: What can we learn from small molecule time resolved?

*Afternoon:* Session 1: Modelling photons in X-ray diffraction Session 2: What is stopping us from publishing?

Friday July 21st

Morning:

How do we move forward with what we've learned? Are we working on the right things? Should we be doing something different here?

### Workshop