Diffraction Methods in Structural Biology 2024

22-27th July 2024

Monday 22nd July	
15-18:30	Arrival and Registration
18:30-20:30	Dinner
20:30-21:30	**The measurement strikes back or the return of the experiment**
We are at a fork in the road, where we have ever more optimised tools for measurement acquisition whilst also developing awesome tools allowing new experiments to be considered: let's consider the capabilities both of these offer in the brave new world of biological crystallography.	
Discussion Leader	Graeme Winter (Diamond Light Source)
Speakers	Nick Pearce (Linköping University)
Tuesday 23rd July	
9:00-10:30	**Development of radiation sources over the last two decades**
Though the development of radiation sources for scattering experiments has been continuous for the full history of crystallography, the last 20 years has seen the "coming of age" of dedicated national and international facilities. How did we get here and how has the experience changed?	
Discussion Leader	Janet Smith (GM/CA, University of Michigan)
Speakers	Katherine McAuley (Paul Scherrer Institute) Clemens Schulz-Briese (DECTRIS, Ltd)
10:30	Break
11:00-13:00	**Making great use of the sources we have today - in many respects we are in a golden age**
What can we do with the spectacular facilities at our disposal? What is possible with the machines we have available today - beyond X-rays, beyond synchrotrons.	
Discussion Leader	Manfred Weiss (Helmholtz Berlin, BESSY)
Speakers	Adrian Mancuso (Diamond Light Source) Dean Myles (ORNL)
13:00-14:00	Lunch
14:00-15:30	**Community challenge discussion 1: handling the data deluge**
16:00	Break
16:30-18:30	Posters & Discussion

18:30	Dinner
20:30-21:30	**Possibilities and challenges afforded by new sources**
While we are in a golden age, there is continuous development and upgrade of the facilities we have access to - what can we and will we do with these tools? What can we usefully do with 1MHz? What can / can't we do with micro beams coupled to very high intensity upgraded sources?	
Discussion Leader	Thomas Schneider (EMBL Hamburg)
Speakers	Yelyzaveta Pulnova (Extreme Light Infrastructure, Prague) Daniele De Sanctis (ESRF)
WEDNESDAY 24TH JULY	
9:00-10:30	**Data processing: how did we get to here?**
Early data processing involved chemicals, later electronic detector technology made this a fully electronic process. Software has evolved from highly interactive to largely automated tools, through the implementation of excellent algorithms and improvements in capturing experiment metadata. Where did this come from?	
Discussion Leader	James Holton (Lawrence Berkeley Laboratory)
Speakers	Kay Diederichs (University of Konstanz) Ana Gonzalez (MAXIV)
10:30	Break
11:00-13:00	**Current interesting topics in data processing**
Though tools have existed for decades to compute spot locations and measure intensities, methods continue to be enhanced and developed, particularly in the area of free electron lasers and serial crystallography - what is the current state of the art?	
Discussion Leader	Jeney Wierman (Cornell)
Speakers	Kevin Dalton (Harvard)
13:00-14:00	Lunch
14:00-15:30	**Community challenge discussion 2: training the next generation**
16:00	Break
16:30-18:30	Posters & Discussion
18:30	Dinner
20:30-21:30	**Future trends and opportunities in the analysis of scattered radiation**

DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024	
Just because the tools we have today are good, does not mean we are doing our best - what more can we extract from the data we acquire in our diffraction experiments? What more can we learn?	
Discussion Leader	Tom White (DESY)
Speakers	Gerhard Hofer (Stockholm) Derek Mendez (SLAC)
THURSDAY 25TH JULY	
9:00-10:30	**Interpretation and use of intensities: a potted history**
The analysis of diffracted intensities and interpretation of patterns is as old as the study of X-ray crystallography - what happened to get us to where we are today?	
Discussion Leader	Gérard Bricogne (Global Phasing)
Speakers	Andrea Thorn (Universität Hamburg)
10:30	Break
11:00-13:00	**Current methods 1: recovering phases and proposing a model**
For decades the phase problem was the biggest challenge in biological crystallography, but the investment in filling the PDB with models has paid off with automated tools for suggesting a model as well as advanced techniques for phasing with and without some prior insight into the structure - what is the best we can do?	
Discussion Leader	Arnaud Basle (University of Newcastle)
Speakers	Saori Maki-Yonekura (RIKEN SPring-8 Center) Lucrezia Catapano (University of Cambridge)
13:00-14:00	Lunch
14:00-15:30	**Discussion**
16:00	Break
16:30-18:30	Posters & Discussion
18:30	Dinner
20:30-21:30	**Current methods 2: optimising agreement between model and measurements**
the initial model is one thing, the best model another - even more important in this time of machine learning based methods. Where have we got in terms of closing the gap between our model and measurements?	
Discussion Leader	Dorothee Liebschner (Lawrence Berkeley Laboratory)

Diffraction Methods in Structural Biology 2024	
Speakers	Alisia Fadini (U Cambridge)
Friday 26th July	
9:00-10:30	**Hypothesis testing as the essence of experiment**
Looking forward we have new opportunities to consider designing experiments to test hypotheses, and develop methods around answering these questions	
Discussion Leader	Ilme Schlichting (MPI-MF)
Speakers	Thomas Barends (MPI-MF)
10:30	Break
11:00-13:00	**Into the fourth (and higher) dimension**
We have spent decades working on static structures as structural biology, but in biology nothing interesting is static, and the process is fascinating - trying to work out how our molecules work. Let's talk about what we can do here looking forwards.	
Discussion Leader	Briony Yorke (University of Leeds)
Speakers	Paulina Dominiak (University of Warsaw) Elke de Zitter (IBS) Martin Fuchs (NSLS II)
13:00-14:00	Lunch
14:00-15:30	**Discussion**
16:00	Break
16:30-18:30	**Posters & Discussion**
18:30	Dinner
Saturday 27th July	
9:00-10:30	**Free/Discussion Time**
10:30	Break
11:00-13:00	**Wrap up: where are we going?**
What are we as a community looking at over the coming couple of years? And hand over to the new chair of the not the GRC.	
Discussion Leader	Kunio Hirata (RIKEN SPring-8 Center)
Speakers	Takahiro Kosugi (National Institutes of Natural Sciences)
13:00-14:00	Lunch
The end!	