

# DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

22-27th July 2024

Note on session timing: both morning sessions have buffer time scheduled to allow discussion - the evening sessions are tight time-wise but we anticipate and look forward to post-session discussion

## MONDAY 22ND JULY

15:00-18:30 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.

Conference Introduction 20:30 - 20:40 **Graeme Winter**

Speakers 20:40 - 21:00 **Nick Pearce** - "Drowning in data: Multi-dataset-driven computational approaches to macromolecular structure determination"  
21:00 - 21:20 **Iris Young** - "Experimenting with new technologies in serial femtosecond crystallography"

# DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

**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?

Session Introduction      09:00 - 09:15 **Janet Smith**

Speakers      09:20 - 09:45 **Katherine McAuley** - "The Evolution of MX Synchrotron Beamlines: Focusing on the Samples"  
09:50 - 10:15 **Clemens Schulze-Briese** - "Towards diffraction limited structural biology"

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.

Session Introduction      11:00 - 11:15 **Manfred Weiss**

Speakers      11:20 - 11:45 **Adrian Mancuso** - "XFELs, Synchrotrons or both? A walk through the complementarity of our large-scale X-ray facilities for diffraction"  
11:45 - 12:10 **Dean Myles** - "Neutron Biophysics: From Atoms to Cells"  
12:10 - 12:35 **Robert Bücker** - "Electron Diffraction in Structural Biology: Chances and Challenges"

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?

Session Introduction      20:30 - 20:40 **Thomas Schneider**

Speakers      20:40 - 21:05 **Daniele de Sanctis** - "Serial Microsecond Crystallography at ESRF-EBS"  
21:05 - 21:30 **Yelyzaveta Pulnova** - "Compact sub-picosecond X-ray plasma source for ultrafast time-resolved diffraction and spectroscopy at ELI Beamlines"

# DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

## 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?

Session Introduction 09:00 - 09:15 **James Holton**

Speakers 09:15 - 09:40 **Ana Gonzalez** "Look ma, no hands!!! Autoprocessing at MX synchrotron beamlines, a brief history and current trends"  
09:45 - 10:10 **Kay Diederichs** - "Data processing: how did we get to here, and where do we go?"

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?

Session Introduction 11:00 - 11:15 **Jeney Wierman**

Speakers 11:20 - 11:45 **Kevin Dalton** - "Scaling Scaling or Stochastic Variational Inference for X-ray Diffraction Data"  
11:45 - 12:10 **Clemens Vornhein** - "Optimising experimental outcomes: improving model construction, refinement, analysis and deposition via better (meta)data handling"  
12:10 - 12:35 **Kunio Hirata** - "Case study of small wedge synchrotron crystallography: Enhancing structural information in micro- and nano-crystals through extensive data collection"

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

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?

Session Introduction 20:30 - 20:40 **Tom White**

Speakers 20:40 - 21:05 **Derek Mendez** - "Modeling the pixels for increased accuracy"  
21:05 - 21:30 **Gerhard Hofer** - "Serial electron diffraction for fast high resolution structure determination"

# DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

**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?

Speakers      09:00 - 09:40 **G rard Bricogne** - "Shepherding diffraction intensities, from birth to resting place."  
09:40 - 10:10 **Elsbeth Garman** - "Diffraction intensity as a radiation damage progression metric and intensity decay models"

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?

Session Introduction      11:00 - 11:15 **Arnaud Basle**

Speakers      11:20 - 11:45 **Saori Maki-Yonekura** - "Measurement of charges and chemical bonding in Cryo-EM SPA"  
11:45 - 12:10 **Lucrezia Catapano** - "Enhancing structural refinement of macromolecules obtained from neutron crystallography"  
12:10 - 12:35 **Andrea Thorn** - "What could be seen in a map without model bias?"

13:00-14:00      Lunch

**14:00-15:30**      **Discussion/Excursions**

16:00      Break/Excursions

**16:30-18:30**      **Posters & Discussion/Excursions**

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?

Session Introduction      20:30 - 20:40 **Dorothee Liebschner**

Speakers      20:40 - 21:05 **Alisia Fadini** - "Teaching OpenFold to Refine Its Predictions with Crystallographic Data"  
21:05 - 21:30 **Florence Tama** - "Phase retrieval software for reconstructing high-resolution, large-volume 3D density maps of biological assemblies"

# DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

## 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

Session  
Introduction

09:00 - 09:20 **Ilme Schlichting**

Speakers

09:20 - 09:45 **Thomas Barends** - "Fantastic Hypotheses and How to Test Them"  
09:45 - 10:10 **Allen Orville** - "Methods and strategies to generalize time-resolved serial MX"

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.

Session  
Introduction

11:00 - 11:15 **Briony Yorke**

Speakers

11:20 - 11:45 **Paulina Dominiak** - "Your data are already four-dimensional! Enhancing three-dimensional spatial representations through the inclusion of electron density and its associated properties"  
11:45 - 12:10 **Martin Fuchs** - "Multiple temperature and time-resolved serial crystallography at NSLS-II"  
12:10 - 12:35 **Elke De Zitter** - "Identifying and modelling low-occupancy states in macromolecular crystallography"

13:00-14:00

Lunch

**14:00-15:30**

**Discussion**

16:00

Break

**16:30-17:45**

**Posters & Discussion**

**17:45-18:30**

**Business Meeting**

18:30

Dinner

## DIFFRACTION METHODS IN STRUCTURAL BIOLOGY 2024

### SATURDAY 27TH JULY

<b>9:00-10:30</b>	<b>Free/Discussion Time</b>
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10:30	Break
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<b>11:00-13:00</b>	<b>Wrap up: where are we going?</b>
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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.

Session Introduction	11:00 - 11:15 <b>Kunio Hirata</b>
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Speakers	11:15 - 11:45 <b>Takahiro Kosugi</b> - "Diffraction Method for Current and Future Protein Design" 11:45 - 12:15 <b>Arwen Pearson</b> - "Quo vadis Diffraction Methods?"
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Organisers	12:15 - 13:00 Meeting Close
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13:00-14:00	Lunch
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THE END!