

CCP4/APS School in Macromolecular Crystallography: From Data Collection to Structure Refinement and Beyond

Argonne National Laboratory

October 28 Monday - November 4 Monday 2024

Virtual Day 1 (Mon 10/7): Bioinformatics

8:00 AM	0:30	Introduction: Outline resources and SLACK Arrangements	
8:30 AM	1:00	Cryo-crystallography	Elspeth Garman
9:30 AM	0:45	Bioinformatics & AlphaFold2	Dan Rigden
10:15 AM	0:15	Break	
10:30 AM	0:45	Generating Your Models (AlphaFold2 and ADB)	Adam Simpkin
11:15 AM	0:45	Assessing Data Quality	Kay Diederichs
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	RoseTTAFold - what's special? TBC	Kathryn Shelley

Virtual day 2 (Mon 10/21): Experimental Data: X-rays and EM

8:00 AM	1:00	Introduction to CCP4	Eugene Krissinel
9:00 AM	1:00	Introduction to symmetry (Space Groups Symmetry and All That)	Charles Ballard
10:00 AM	0:15	Break	
10:15 AM	1:00	Introduction to data processing	David Waterman
11:15 AM	0:45	On Visiting APS and GMCA Resources	
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	How to Collect the Best Macromolecular Diffraction Data - Dectris	Sofia Trampari
2:00 PM	1:00	Mitegen	Joyce Frank
2:00 PM	1:00	Overview Cryo EM	TBA

Day 1 (Mon 10/28): Data Collection and Processing

8:00 AM	0:15	Welcome and Introduction	Qingping Xu
8:15 AM	1:00	Basic Diffraction Theory	Kamel El Omari
9:15 AM	0:45	Data Collection Concepts	Ruslan Sanishvili (Nukri)
10:00 AM	0:15	Break	
1:00 PM	1:00	Data Collection: Strategies, Practical Tips	Ruslan Sanishvili (Nukri)
11:15 AM	0:45	Data Processing with DIALS - demo-lecture	Graeme Winter
12:00 AM	1:00	Lunch break	
1:00 PM	0:45	Data Processing with HKL3000 - demo-lecture	Dominika Borek
1:45 PM	0:45	Data Processing with XDS - demo-lecture	Kay Diederichs
2:30 PM	0:15	Break	
2:45 PM	0:45	Sector Orientation and Beamline Tour	Naga Venugopalan
3:30 AM	1:00	Data Collection Planning	TBA
4:30 PM	1:00	Student Presentations Part 1 + beer	Students
5:30 PM	0:15	Break	
5:45 PM	1:15	Student Presentations Part 2 + beer	Students

7:00 PM	1:00	Dinner Break	
8:00 PM	2:00	Beer or Practical Session	

Day 2 (Tue 10/29): Data Collection and Processing // EM Relion SPA tutorial

8:00 AM	24:00	X-ray Data Collection	Qingping Xu <i>et al.</i>
8:00 AM	1:00	Radiation Damage	Elspeth Garman
9:00 AM	3:00	EM Relion SPA tutorial	Joel Greer, Paul Emsley <i>et al.</i>
12:00 PM	1:00	Lunch Break	
1:00 PM	2:30	EM Relion SPA tutorial	Joel Greer, Paul Emsley <i>et al.</i>
3:30 PM	1:00	New tomography tools in Relion5/Dopio	Rangana Warshamanage, CCPEM (remote)
4:30 PM	2:30	EM Relion SPA tutorial and Practical Session	Joel Greer, Paul Emsley <i>et al.</i>
7:00 PM	1:00	Dinner Break	
8:00 PM	2:00	Practical Session	Joel Greer, Paul Emsley <i>et al.</i>

Day 3 (Wed 10/30): Data Processing and Experimental Phasing

8:00 AM	1:30	Scaling and Merging the Data (Multi-crystal Data)	Graeme Winter
9:30 AM	1:00	Twinning and Other Pathologies lecture + demo	Andrey Lebedev (Virtual)
10:30 AM	1:00	CCP4 Cloud: key concepts and data upload	CCP4
11:30 AM	0:30	Coot and Moorhen Introduction + setup debugging	CCP4
12:00 PM	1:00	Lunch Break	
1:00 PM	4:30	Processing Data	
5:30 PM	1:00	Phase Problem + EP	Ed Lowe (Virtual)
6:30 PM	0:30	Phasing Demo EP	Ed Lowe (Virtual)
7:00 PM	1:00	Dinner Break	
8:00 PM	1:00	Experimental Phasing: Long Wavelength, Soaks, Identification of Metals	Kamel El'Omari
9:00 PM	1:00	Dataset of the Day and Practical Session	

Day 4 (Thu 10/31): Molecular Replacement

8:00 AM	1:00	Molecular Replacement - basics	Randy Read (Virtual)
9:00 AM	1:00	Phaser, model prep, docking into CryoEM lectures	Randy Read (Virtual)
10:00 AM	0:15	Break	
10:15 AM	1:00	MR in CCP4 Talk/Demo	Ronan Keegan
11:15 AM	0:45	Alpha Fold everywhere	Oleg Kovalevskiy (Virtual)
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	Arcimboldo, Shelx for MR	Josep Triviño
2:00 PM	1:00	Phasing in Phenix	Dorothee Liebschner
3:00 PM	4:00	Practical Session	
7:00 PM	1:00	Dinner Break	
8:00 PM	2:00	Dataset of the Day and Practical Session	

Day 5 (Fri 11/1): Model Building

8:00 AM	1:00	Intro to model building and model building in COOT	Paul Emsley
9:00 AM	1:00	Model Building in Phenix	Dorothee Liebschner
10:00 AM	0:15	Break	
10:15 AM	0:45	ARP/wARP	Grzegorz Chojnowski
11:00 PM	1:00	Automatic model building in CCP4: Modelcraft.	Paul Bond
12:00 PM	1:00	Lunch	
1:00 PM		Free time (afternoon and evening)	

Day 6 (Sat 11/2): Refinement and Ligands

8:00 AM	0:45	Intro to Refinement with CCP4	Rob Nicholls
8:45 AM	1:00	Examples on model-building errors	Robbie Joosten
9:45 PM	0:15	Break	
10:00 AM	1:00	Modelling ligands in CCP4	Rob Nicholls
11:00 AM	1:00	Refinement against cryoEM reconstructions	Rob Nicholls
12:00 PM	1:00	Lunch Break	
1:00 PM	1:30	Phenix-refine	Pavel Afonine
2:30 PM	4:30	Practical Session	
7:00 PM	1:00	Dinner Break	
8:00 PM	2:00	Dataset of the Day and Practical Session	

Day 7 (Sun 11/3): Other Macromolecules, Ligands, Validation

8:00 AM	1:00	Carbohydrates	Jon Agirre (Virtual)
9:00 AM	0:45:	Coot advanced including DNA/RNA and ligands	Paul Emsley
9:45 AM	0:15	Break	
10:00 AM	0:45	Coot advanced including DNA/RNA and ligands	Paul Emsley
10:45 AM	1:15	Model completion and Validation	Robbie Joosten
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	Validation in Phenix	Pavel Afonine
2:00 PM	5:00	Practical Session	
7:00 PM	1:00	Dinner Break	
8:00 PM	2:00	Dataset of the Day and Practical Session	

Day 8 (Mon 11/4): Structure Analysis and Deposition

8:00 AM	1:00	CryoEM: Tools in Phenix	Pavel Afonine
9:00 AM	1:00	Cryo-EM: Model Fitting and Validation	Grzegorz Chojnowski
10:00 AM	0:15	Break	
10:15 AM	1:00	Raddam TBC	Kathryn Shelley
11:15 AM	0:45	RCSB tools (PDB 101 etc) and PDB deposition	Brian Hudson (Virtual)
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	Structural Analysis & Macromolecular Complexes	Eugene Krissinel (Virtual)
2:00 PM	2:00+	The last hands on and backup	
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