

CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond

Argonne National Laboratory

March 27 - April 3, 2023

All Lectures will be held in the Conference Center of Advanced Protein Characterization Facility, Building 446. All meals and refreshments will be arranged in the next room from the Conference Center, except for dinner on Monday the 27th, and all meals and refreshments on Tuesday, March 28. These will be served in the conference room C010 of Building 436.

3/6/2023 (day 0)

Cryo and bioinformatics

Virtual

8:00:00 AM CST		Intro: outline and tools
	25'	point to: CCP4 Cloud, phenix, xds,
	60'	slack arrangements
	45'	Cryocrystallography
		Bioinformatics & AlphaFold
		Break
	45'	Generating your models (AlphaFold and ADB)
	45'	On visiting APS/GMCA resources
	60'	Lunch break
	60'	Student presentations
	15'	Break
	60'	Student presentations

3/27/2023 (day 1)

Data collection

Building 446 Auditorium

8:00:00 AM CST	15'	Welcome and Introduction
	60'	Basic Diffraction Theory
	60'	Data Collection Strategies
	15'	Break
		Multicrystal
	60'	practical aspects + touch scaling as well
	60'	Assesing your data
	15'	Lunch break
	45'	Data Processing with DIALS - demo-lecture
	45'	Data Processing with HKL300 - demo-lecture
	15'	Break
	45'	Data Processing with XDS - demo-lecture
19:00:00 PM	30'	Sector Orientation
	30'	Beamline tour
	60'	Dinner break
	60'	Data collection planning

3/28/2023 (day 2)

Data collection and processing

Beamlines 23ID-B and 23ID-D

9:00:00 AM CST	30'	Coot introduction (informal, conf room Blg 436, next to beamline 23 IDB)
	30'	CCP4 cloud introduction (informal, conf room Blg 436, next to beamline 23 IDB)
10:00:00	120'	Data collection
12:00:00	60'	Lunch break
1:00:00	360'	Data collection
19:00:00 PM	60'	Dinner break
20:00:00	240'	Data collection

3/29/2023 (day 3)

Twinning; Data processing and tutorials

Building 446 Auditorium

8:00:00	60'	Space groups, symmetry, and all that
	45' +	
	15' break	Scaling and merging the data
	+ 45'	also multicrystal
	15'	Break
	90'	Twinning and other pathologies,
		practical aspects + demo
12:00:00	60'	Lunch break
13:00:00	60'	Intro to CCP4
14:00:00	300'	Processing data
19:00:00	60'	Dinner break
20:00:00	120'	Dataset of the day

3/30/2023 (day 4)

Phasing (Exp Phasing & Molecular replacement)

Building 446 Auditorium

08:00 - 09:00	45'	Phase problem
	45'	intro exp phasing + DM
	45'	Molecular replacement
	15'	Break
	45'	MR-SAD concept - short
	45'	MR - Assessing and improving
	60'	the solution
		Lunch break
	45'	Advanced MR "tricks" Michail Isupov
		includes: model prep
	45'	Phasing in CCP4 - demo
		(includes: Arcimboldo, Shelx for mr, CCP4mg)
	60'	Exp Phasing in Phenix - lecture + demo (MR in Phenix)
19:00:00	60'	Dinner break
20:00:00	120'	Dataset of the day and Practical session

3/31/2023 (day 5)

Model Building

Building 446 Auditorium

8:00:00	60'	Model building in Phenix
	45'	ARP/wARP
	15'	Break
	60'	TBD
	45'	Model building in CCP4 - Modelcraft, Nautilus
12:00:00	60'	Lunch
13:00:00		Afternoon and evening: free time

4/1/2023 (day 6)

Refinement and Autobuilding

Building 446 Auditorium

8:00:00	60'	refmac + restraints + dictionaries + low/high reso ref
	45'	refmac - continued
	15'	Break
	60'	phenix-refine
	60'	coot tools for model building
12:00:00	60'	Lunch break
13:00:00	360'	Practical session
19:00:00	60'	Dinner break
20:00:00	120'	Dataset of the day and practical session

4/2/2023 (day 7)

Ligands and validation

Building 446 Auditorium

8:00:00	45'	DNA/RNA
	45'	Carbohydrates
	15'	Break
	45'	Ligands and ligand dictionaries (lecture + tutorial)
	60'	Validation (lecture + tutorial)
12:00:00	60'	Lunch break
	60'	Validation in Phenix (lecture w tutorial)
19:00:00	60'	Dinner break
20:00:00	120'	Dataset of the day and practical session

4/3/2023 (day 8)

Structure Analysis, EM and Feedbacks

Building 446 Auditorium

8:00:00	60'	Radiation damage
	60'	Molecular graphics for analysis & publications
	60'	Structural analysis & Macromolecular Complexes
	15'	Break
	60'	Deposition
	60'	EM
	60'	Lunch break

The last hands on
Backup

Aurevoire

Name	Affiliation	Email	Available?
Pavel Afonine	Lawrence Berkeley Laboratory, California, USA		y
Charles Ballard	STFC Rutherford Appleton Laboratory, UK		y
Dominika Borek	Southwestern Medical Center, Dallas, USA		y
Grzegorz Chojnowski	EMBL, Hamburg, Germany		
Kay Diederichs	University of Konstanz		y -provisional
Robert Fischetti	Argonne National Laboratory, USA		
Andreas Forster	Dectris Ltd., Switzerland (suggested remote)		
Brian Hudson	RCSB, USA		y - remote
Robbie Joosten	Netherlands Cancer Institute, Amsterdam, The Netherlands		y
Eugene Krissinel	STFC Rutherford Appleton Laboratory, UK		y
Andrey Lebedev	STFC Rutherford Appleton Laboratory, UK		y
Paul Emsley	MRC-LMB, Cambridge, UK		y -provisional
Dorothee Liebschner	Lawrence Berkeley Laboratory, California, USA		y
Edward Lowe	Oxford University, UK		y -provisional
Ruslan Sanishvili	Argonne National Laboratory, Argonne, USA		y -provisional
Paul Bond	York University, UK		to ask??
Rob Nicholls or Ketaro	MRC Laboratory of Molecular Biology, UK		y -provisional
David Waterman	DLS, Oxford, UK		y -provisional
Graeme Winter	DLS, Oxford, UK		y -provisional
Rob Offener			
Michail Isupov			y -provisional
Elspeth			invite
Adam Simpkin			
Dan Rigden			
Ronan			
Maria			
Raj			??