

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

Argonne National Laboratory

June 17 - 24, 2019

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 18th, and all meals and refreshments on Tuesday, June 19. These will be served in the conference room C010 of Building 436.

Color code:

Meal or Coffee break

Lecture session

Practical session

Tutorial session

Other

Speakers:

Pavel Afonine	Lawrence Berkeley Laboratory, California, USA
Charles Ballard	STFC Rutherford Appleton Laboratory, UK
Dominika Borek	Southwestern Medical Center, Dallas, USA
Grzegorz Chojnowski	EMBL, Hamburg, Germany
Kay Diederichs	University of Konstanz
Robert Fischetti	Argonne National Laboratory, USA
Andreas Forster	Dectris Ltd., Switzerland
Brian Hudson	RCSB, USA
Robbie Joosten	Netherlands Cancer Institute, Amsterdam, The Netherlands
Eugene Krissinel	STFC Rutherford Appleton Laboratory, UK
Andrey Lebedev	STFC Rutherford Appleton Laboratory, UK
Paul Emsley	MRC-LMB, Cambridge, UK
Dorothee Liebschner	Lawrence Berkeley Laboratory, California, USA
Edward Lowe	Oxford University, UK
Stuart McNicholas	York University, UK
Ethan Merritt	University of Washington, USA
Ruslan Sanishvili	Argonne National Laboratory, Argonne, USA
Paul Bond	York University, UK
Rob Nicholls	MRC Laboratory of Molecular Biology, UK
Massimo Sammito	CIMR, University of Cambridge, UK
James Beilsten-Edmands	DLS, Oxford, UK
Graeme Winter	DLS, Oxford, UK

Monday, 17th June

Introduction; Data collection and processing lectures; Beamline training; data collection planning; Registration.

08:00 - 08:45	Breakfast	Building 446
08:45 – 09:00	Welcome and Introduction	B. Fischetti and Q Xu, Building 446
09:00 – 09:45	GM/CA Overview, Serial Crystallography & APS-U	B. Fischetti, Building 446
09:45 – 10:30	MX diffraction data collection	R. Sanishvili, Building 446
10:30 – 11:15	Optimizing data quality with Hybrid Photon Counting detectors	A. Förster, Building 446
11:15 – 12:00	Data processing with HKL	D. Borek, Building 446
12:00 – 12:45	Lunch	Building 446
12:45 – 13:45	Data Processing with DIALS	G. Winter, Building 446
13:45 – 14:45	Data processing with XDS	K. Diederichs, Building 446
14:45 – 15:15	Good data with XDS, data quality indicators	K. Diederichs, Building 446
15:15 – 15:30	Break. Walk to the sector 23	All students with crystals. The rest are optional
15:30 – 16:00	Sector Orientation	M. Becker, Bld. 436, Sector 23
16:00 – 16:30	Beamline tour	S. Corcoran Bld. 436, Sector 23
16:30 – 18:00	Hands on training on Beamline Controls and Data Collection Software	GMCA staff, Beamlines 23ID-B and 23ID-D
18:00 – 19:00	Data collection planning	All participants Building 436, C010
19:00 – 20:00	Dinner Q&A session.	All participants. Building 436, C010

20:00 – 21:00	Prepare Samples	GM/CA staff GMCA Lab
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Tuesday, 18th June

Data collection and processing

Beamlines 23ID-B and 23ID-D

08:00 – 09:00	Beamline setup	GM/CA staff Beamlines 23ID-D and 23ID-B
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08:00 - 09:00	Breakfast	Building 436, conference room C010
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09:00 – 12:00	Data collection and real-time processing	GM/CA staff, D. Borek, G. Winter, K. Diederichs
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12:00 – 12:45	Working Lunch with continued data collection and processing (Q&A session)	All participants Building 436, conference room C010
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12:45 – 16:00	Data collection and real-time processing	GM/CA staff, D. Borek, G. Winter, K. Diederichs
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16:00 – 16:30	Break	
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16:30 – 19:00	Data collection and real-time processing	GM/CA staff, D. Borek, G. Winter, K. Diederichs
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19:00 – 20:00	Dinner	Building 436, conference room C010
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20:00 – 24:00	Data collection and real-time processing	GM/CA staff, D. Borek, G. Winter, K. Diederichs
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Wednesday, 19th June

***Overview of student's crystallographic problems;
Twinning; Data processing and tutorials***
Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 10:00	Scaling and merging the data	J. Beilsten-Edmands
10:00 – 11:00	Space groups, symmetry and all that	C. Ballard
11:00 – 12:00	Twinning and other pathologies, practical aspects	A. Lebedev
12:00 – 12:45	Lunch	
12:45 - 13:15	Overview of crystallographic problems	All participants
13:15 – 14:45	Processing with HKL. Student data	D. Borek
14:45 – 16:15	Processing with DIALS. Student data	D. Waterman
16:15 – 16:30	Break	
16:30 – 18:00	Processing with XDS. Student data	K. Diederichs
18:30 – 19:30	Data processing	All participants
19:30 – 20:30	Dinner	
20:30 – 22:00	Data processing	All participants

Thursday, 20th June

Overview of CCP4; Experimental phasing; Finish data processing

Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
9:00 – 09:45	Introduction to CCP4	E. Krissinel
9:00 – 10:30	Introduction to phasing	E. Lowe
10:30 – 11:15	SHELXC/D/E	M. Sammito
11:15 – 12:00	Phasing and automation in Phenix	D. Liebschner
12:00 – 12:45	Lunch	
12:45 – 13:30	Experimental Phasing with Phaser	E. Lowe
13:30 – 14:15	Density modification	P. Bond
14:15 – 14:30	Tutorial Crank/Crank 2 introduction	
14:30 – 14:45	Tutorial Pirate Buccaneer introduction	
14:45 – 15:00	Tutorial SHELXC/D/E	
15:00 – 15:15	Tutorial Phenix - experimental phasing	D. Liebschner
15:15 – 15:30	Tutorial Phaser EP	E. Lowe
15:30 – 15:50	Break	
15:50 – 19:00	Hands-on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands-on problem solving	All participants

Friday, 21st June

Molecular replacement

Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:50	Introduction to Phaser-MR	M. Sammito
09:50 – 10:30	Model Preparation for MR and assessing the solution	A. Lebedev
10:30 – 11:10	MR pipelines	A Lebedev
11:10 – 11:35	SHELXE for Molecular Replacement, and ARCIMBOLDO pipelines	M. Sammito
11:35 – 12:00	Building with buccaneer and nautilus	P. Bond
12:00 – 12:45	Lunch	
12:45 – 13:00	Tutorial: Molecular Replacement	A. Lebedev
13:00 – 13:15	Tutorial: Phaser MR	M. Sammito
13:15 – 13:30	Tutorial: MR in CCP4MG	S. McNicholas
13:30 – 13:45	Tutorial: Automated MR	A. Lebedev
13:45 – 14:00	Tutorial: SHELX	T. Gruene
14:00 –	Afternoon and evening: free time	

Saturday, 22nd June

Refinement and Autobuilding

Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:45	Refmac	R. Nicholls
09:45 – 10:30	Phenix refinement and ligand building	P. Afonine
10:30 – 11:15	TLS and all that	E. Merritt
11:15 – 12:00	Automated Protein Model Building with ARP/wARP 8.0	G. Chojnowski
12:00 – 12:45	Lunch	
12:45 – 13:15	Coot: An Introduction	P. Emsley
13:15 – 13:45	CCP4MG: Introduction	S. McNicholas
13:45 – 14:00	Tutorial: Refmac	R. Nicholls
14:00 – 14:15	Tutorial: Phenix - refinement	P. Afonine
14:15 – 14:45	Tutorial: TLS	E. Merritt
14:45 – 15:00	Tutorial: Classic Model Building in ARP/wARP	G. Chojnowski
15:00 – 15:15	Tutorial: Coot	P. Emsley
15:15 – 16:15	Hands on problem solving	All participants
16:15 – 16:30	Break	
16:30 – 19:00	Hands on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands on problem solving	All participants

Sunday, 23rd June

Ligands and validation

Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
9:00 – 9:30	Ligands and ligand dictionary	R.Nicholls
9:30 – 10:00	Automatic Building of Ligands and Nucleotides in ARP/wARP 8.0	G. Chojnowski
10:00 – 10:40	Coot ligand building	P. Emsley
10:40 – 11:20	Validation in Phenix	P. Afonine
11:20 – 12:00	How good is my model and can it be improved?	R. Joosten
12:00 – 12:45	Lunch	
12:45 – 13:30	wwPDB OneDep tools for deposition and validation	B. Hudson
13:30 – 13:45	Tutorials: Ligands and ligand dictionary	R. Nicholls
13:45 – 14:00	Tutorials: Automatic Building of Ligands and Nucleotides in ARP/wARP	G. Chojnowski
14:00 – 14:15	Tutorial: Coot ligand building	P. Emsley
14:15 – 14:30	Tutorial: PDB-REDO and validation	R. Joosten
14:30 – 16:00	Hands on problem solving	All participants
16:00 – 16:30	Break	
16:30 – 19:00	Hands on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands on problem solving	All participants

Monday, 24th June

Structure Analysis, Molecular Graphics and Feedback

Building 446 Auditorium

08:00 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:20	CCP4 beyond structure solution	E. Krissinel
09:20 – 10:00	Analysis of macromolecular Complexes (PISA)	E. Krissinel
10:00 – 10:45	CCP4mg – Advanced options Demo and tutorial	S. McNicholas
10:45 – 11:30	An introduction to single particle cryo-EM	R. Nicholls
11:30 – 12:00	Start backups	All participants
12:00 – 12:45	Lunch	
12:45 – 16:00	Hands on problem solving	All participants
16:00 – 16:15	Break	
16:15 – 17:30	Hands on problem solving	All participants
17:30 – 19:30	Overview of crystallographic problems and backups	All participants
19:30 – 19:40	Concluding remarks	Organizers
19:40 – 20:40	Dinner	

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