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

Argonne National Laboratory

June 18 - 25, 2018

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:

David Waterman (STFC, UK) -- DIALS data processing package

Kay Diederichs (Konstanz, Germany) -- XDS data processing, data quality indicators, **good data with xds,** non-isomorphism of data, serial crystallography

Tim Gruene (PSI, Switzerland) -- SHELX, electron diffraction

Dominika Borek (Texas SouthWestern) [APS invite] -- available for 2018

Andrey Lebedev (STFC, UK) -- CCP4

Raj Pannu (Leiden, Nederlands) -- CRANK, experimental phasing

Dorothee Leibschner (LBNL) -- phenix

Pavol Afonine (LBNL) -- phenix

Ethan Merritt (Washington) -- TLS

Eugene Krissinel (STFC) -- CCP4

Massimo Sammito (Cambridge, UK) -- phaser, ARCIMBOLDO

Rob Nichols (LMB-MRC) -- refinement, ligands

Grzegorz Chojnowski (Hamburg) -- Arp/Warp

Bernhard Lohkamp (Uppsala, Sweden) -- COOT

Robbie Joosten (NKI, Nederlands) -- PDB redo, refinement

K. Rajashankar (NECAT/APS)

B Hudson (RCSB/wwPDB) -- PDB

Charles Ballard (STFC, UK) -- CCP4

Ed Lowe (Oxford) -- EP and general

Stuart McNicholas (York, UK) -- CCP4MG

What follows is 2017 with dates amended

Monday, 18th June

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

08:00 – 08:30	**Welcome and Introduction**	B. Fischetti and Q Xu, *Building 446*
08:30 - 09:00	Breakfast	*Building 446*
09:00 – 09:45	**General overview: synchrotron radiation & beamline etc TBD**	B. Fischetti, *Building 446*
09:45 – 10:15	**Data collection and quality TBD**	K. Rajashankar, *Building 446*
10:15 – 11:00	**TBC**	TBC, *Building 446*
11:00 – 12:00	**Data processing with HKL**	D. Borek, *Building 446*
12:00 – 12:45	Lunch	*Building 446*
12:45 – 13:45	**DIALS and BLEND**	D. Waterman, *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**	S. Corcoran, *Bld. 436, Sector 23*
16:00 – 16:30	**Beamline tour**	V. Nagarajan *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*

Tuesday, 19th 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*
08:30 - 09:00	Breakfast	*Building 436, conference room C010*
09:00 – 12:00	**Data collection and real-time processing**	GM/CA staff, D. Borek, D. Waterman, K. Diederichs
12:00 – 12:45	Working Lunch with continued data collection and processing (Q&A session)	All participants *Building 436, conference room C010*
12:45 – 16:00	**Data collection and real-time processing**	GM/CA staff, D. Borek, D. Waterman, K. Diederichs
16:00 – 16:30	Break	
16:30 – 19:00	**Data collection and real-time processing**	GM/CA staff, D. Borek, D. Waterman, K. Diederichs
19:00 – 20:00	Dinner	*Building 436, conference room C010*
20:00 – 24:00	**Data collection and real-time processing**	GM/CA staff, D. Borek, D. Waterman, K. Diederichs

Wednesday, 20st June

Overview of student's crystallographic problems; Twinning; Data processing and tutorials

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
09:00 – 10:00	**Overview of crystallographic problems**	All participants
10:00 – 11:00	**Scaling and spacegroups**	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, continued**	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, 21st June

Overview of CCP4; Experimental phasing; Finish data processing

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
9:00 – 09:45	**Introduction to CCP4**	E. Krissinel
9:00 – 10:30	**Experimental Phasing & Crank/Crank2**	R. Pannu
10:30 – 11:15	**SHELXC/D/E**	T. Gruene
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	**Parrot/Buccaneer**	B. Lohkamp
14:15 – 14:30	**Tutorial Crank/Crank 2**	R. Pannu
14:30 – 14:45	**Tutorial Pirate Buccaneer**	B. Lohkamp
14:45 – 15:00	**Tutorial SHELXC/D/E**	T. Gruene
15:00 – 15:15	**Tutorial Phenix**	T. Terwilliger
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, 22nd June

Molecular replacement

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
09:00 – 09:50	**Introduction to Phaser-MR and ARCIMBOLDO**	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**	T. Gruene
11:35 – 12:00	**Structural Biology with Electron Diffraction**	T. Gruene
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, 23rd June

Refinement and Autobuilding

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
09:00 – 09:45	**Refmac**	R. Nichols
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 7.4**	G. Chojnowski
12:00 – 12:45	Lunch	
12:45 – 13:15	**Coot: An Introduction**	B. Lohkamp
13:15 – 13:45	**CCP4MG: Introduction**	S. McNicholas
13:45 – 14:00	**Tutorial: Refmac**	R. Nichols
14:00 – 14:15	**Tutorial: Phenix**	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**	B. Lohkamp
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, 24th June

Ligands and validation

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
9:00 – 9:30	**Ligands and ligand dictionary**	R.Nichols
9:30 – 10:00	**Automatic Building of Ligands and Nucleotides in ARP/wARP 7.4**	G. Chojnowski
10:00 – 10:40	**Coot ligand building**	B. Lohkamp
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**	G. Murshudov
13:45 – 14:00	**Tutorials: Automatic Building of Ligands and Nucleotides in ARP/wARP**	G. Chojnowski
14:00 – 14:15	**Tutorial: Coot ligand building**	B. Lohkamp
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, 25th June

Structure Analysis, Molecular Graphics and Feedback

Building 446 Auditorium

08:30 - 09:00	Breakfast	*Building 446*
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. Nicholas
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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