

Diamond-CCP4 Data Collection & Structure Solution Workshop 2022

Before fishing crystals

Talks	Mon 17th October	
Practical	AM CHAIR:	
Break	8:30	
Social	8:45	
	9:00	
	9:15	
	9:30	
	9:45	Informal hello/meet & greet
	10:00	MX at Diamond
	10:15	Marco Mazzorana
	10:30	
	10:45	Navigating Diamond SynchWeb - video to send in advance
	11:00	
	11:15	Marco Mazzorana
	11:30	
	11:45	login to synchweb check
	12:00	
	12:15	
	12:30	Lunch
	12:45	
	PM CHAIR:	
	13:00	Optimising the Diamond experience
	13:15	David Lawson
	13:30	
	13:45	Cryocrystallography
	14:00	Elspeth Garman
	14:15	
	14:30	Generating predicted models for MR
	14:45	Adam Simpkin
	15:00	
	15:15	Running alphafold at DLS - Elliot Nelson
	15:30	
	15:45	Navigating the Diamond cluster
	16:00	Felicity Bertram
	16:15	
	16:30	follow up Fed ID problems
	16:45	
	17:00	

Online setup day

Tue 22nd November	
AM CHAIR:	
8:30	
8:45	
9:00	
9:15	
9:30	Informal hello/meet & greet
9:45	Welcome & introduction to CCP4
10:00	Eugene Krissinel
10:15	Introduction to CCP4 interfaces
10:30	(Cloud/ccp4i2) - setup accounts and run tutorial data
10:45	
11:00	Eugene Krissinel / Andrey Lebedev
11:15	Break
11:30	
11:45	Basic Diffraction Theory
12:00	Kamel El Omari
12:15	
12:30	
12:45	Lunch
13:00	
PM CHAIR:	
13:15	Data Collection Strategies for Photon Counting Detectors
13:30	
13:45	Graeme Winter
14:00	Radiation damage
14:15	Elspeth Garman
14:30	
14:45	Dose driven data collection to optimise your experiments
15:00	
15:15	David Aragão
15:30	Break
15:45	
16:00	Data Processing (inc scaling)
16:15	Ana Gonzalez
16:30	
16:45	
17:00	

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Week 1: data collection and processing, phasing

Data collection

Data processing

Experimental phasin

Molecular replacement

MR / model building

Talks	Sun 27th November	Mon 28th November	Tue 29th November	Wed 30th November	Thu 1st December	Fri 2nd December
Practical	ARRIVAL	BEAMLINE DAY	AM CHAIR: David Waterman	AM CHAIR: Felicity Bertram	AM CHAIR: Emily Cross	AM CHAIR: David Waterman
Break		8:15 X32 08:15 bus	8:15 X32 08:15 bus	8:15 X32 08:15 bus	8:15 X32 08:15 bus	8:15 X32 08:15 bus
Social		8:30	8:30	8:30	8:30	8:30
		8:45 X32 08:48 bus	8:45 X32 08:48 bus	8:45 X32 08:48 bus	8:45 X32 08:48 bus	8:45 X32 08:48 bus
		9:00	9:00	9:00	9:00	9:00
		9:15 Practical guide for data collection at Diamond	9:15 XDS (demo/tutorial) Kay Diederichs	9:15 An introduction to Coot Judit Debreczeni	9:15 Bioinformatics for structural biologists Dan Rigden	9:15 MR - Assessing and improving the solution Ronan Keegan
		9:30		9:30	9:30	9:30
		9:45 Marco Mazzorana		9:45	9:45	9:45
		10:00	10:00	10:00 Pathologies and pseudosymmetry	10:00 Molecular replacement	10:00 MR case studies
		10:15	10:15	10:15	10:15	10:15
		10:30	10:30	10:30	10:30	10:30
		10:45	10:45	10:45	10:45	10:45
		11:00	11:00	11:00	11:00	11:00
		11:15	11:15	11:15	11:15	11:15
		11:30	11:30	11:30	11:30	11:30
		11:45	11:45	11:45	11:45	11:45
		12:00	12:00	12:00	12:00	12:00
		12:15	12:15	12:15	12:15	12:15
		12:30	12:30	12:30	12:30	12:30
		12:45	12:45	12:45	12:45	12:45
			PM CHAIR: Ramona Duman	PM CHAIR: Christian Orr	PM CHAIR: Ramona Duman	PM CHAIR: Ronan Keegan
		13:00	13:00	13:00	13:00	13:00
		13:15	13:15	13:15	13:15	13:15
		13:30	13:30	13:30	13:30	13:30
		13:45	13:45	13:45	13:45	13:45
		14:00	14:00	14:00	14:00	14:00
		14:15	14:15	14:15	14:15	14:15
		14:30	14:30	14:30	14:30	14:30
		14:45	14:45	14:45	14:45	14:45
15:00	Arrive at The Bear, Wantage	15:00	15:00	15:00	15:00	
15:15		15:15	15:15	15:15	15:15	
15:30		15:30	15:30	15:30	15:30	
15:45		15:45	15:45	15:45	15:45	
16:00		16:00	16:00	16:00	16:00	
16:15		16:15	16:15	16:15	16:15	
16:30		16:30	16:30	16:30	16:30	
16:45		16:45	16:45	16:45	16:45	
17:00		17:00	17:00	EVENING CHAIR: Felicity Bertram		17:00
17:15		17:15	17:15	17:15	17:15	17:15
17:30		17:30	17:30	17:30	17:30	17:30
17:45		17:45	17:45	17:45	17:45	17:45
18:00		18:00	18:00	18:00	18:00	18:00
18:15		18:15	18:15	18:15	18:15	18:15
18:30		18:30	18:30	18:30	18:30	18:30
18:45		18:45	18:45	18:45	18:45	18:45
19:00	19:00	19:00	19:00	19:00	19:00	
19:15	19:15	19:15	19:15	19:15	19:15	
19:30	19:30	19:30	19:30	19:30	19:30	
19:45	19:45	19:45	19:45	19:45	19:45	
20:00	20:00	20:00	20:00	20:00	20:00	
20:15	20:15	20:15	20:15	20:15	20:15	

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Week 2: model building, refinement and validation

Model building / refinement

Model building / validation

Wrap u

Talks	Sat 3rd December	Sun 4th December	Mon 5th December	Tue 6th December	
Practical	Free day	AM CHAIR: Christian Orr	AM CHAIR: José Brandão-Neto	AM CHAIR: Anna Warren	
Break		8:00	8:00	8:00	
Social		8:15	X32 08:15 bus	8:15 X32 08:15 bus	
		8:30	8:30	8:30	
		8:45	X32 08:48 bus	8:45 X32 08:48 bus	
		9:00	9:00	9:00	
		9:15	Coach from The Bear	9:15	
		9:30	DM Robbie Joosten	9:30	MX from an Industrial Perspective Ailsa Powell
		9:45		9:45	
		10:00	New developments in model building and validation Grzegorz Chojnowski	10:00	CCP4MG practical Stuart McNicholas
		10:15		10:15	
		10:30	10:30		
		10:45	10:45		
		11:00	Break	11:00	Break
		11:15	Refinement Lucrezia Catapano	11:15	Future of structural biology Michael Zahn
		11:30		11:30	
		11:45	Announce Poster Session Winner	11:45	
		12:00	Beamline specific talk	12:00	
		12:15	Lunch	12:15	Beamline specific talk
		12:30		12:30	Lunch
		12:45		12:45	
			PM CHAIR: Dave Hall	PM CHAIR: Maria Fando	13:00
		13:00	REFMAC tutorial Robert Nicholls	13:00	PM CHAIRS:
		13:15		13:15	
		13:30	Refinement case studies Clemens Vornrhein	13:30	Student feedback session - 5 min presentations
		13:45		13:45	
		14:00	Work on your own data	14:00	
		14:15		14:15	
		14:30		14:30	
		14:45	14:45	14:45	Break
		15:00	Work on your own data	15:00	
		15:15		15:15	
		15:30	Break	15:30	
		15:45	15:45	15:45	
		16:00		16:00	Wrap up from organisers
		16:15		16:15	
		16:30		16:30	
		16:45		16:45	
		17:00		17:00	
		17:15	Dataset of the day All tutors	17:15	
		17:30		17:30	
		17:45		17:45	
		18:00	Dinner	18:00	
		18:15		X32 18:21 bus	18:15
		18:30			18:30
		18:45		X32 18:53 bus	18:45
		19:00		19:00	
		19:15		19:15	
		19:30		19:30	
		19:45		19:45	
	20:00	20:00			
	20:15	20:15			
	Coach to The Bear				