

Diamond-CCP4 Data Collection & Structure Solution Workshop 2023

Zoom day 1: before fishing crystals

Talks		Mon 6th November	
Practical		AM CHAIR: Hans Pfalzgraf	
Break	8:30		
Social	8:45		
	9:00		
	9:15		
	9:30		
	9:45	Informal hello/meet & greet	
	10:00	MX at Diamond Marco Mazzorana	
	10:15		
	10:30		
	10:45	Navigating Diamond SynchWeb - Marco	
	11:00	login to synchweb check	
	11:15		
	11:30		
	11:45	Optimising the Diamond experience David Lawson	
	12:00	Lunch	
	12:15		
	12:30		
	12:45		
		PM CHAIR: Adam Crawshaw	
	13:00	Cryocrystallography Elspeth Garman	
	13:15		
	13:30		
	13:45	Advanced MX at VMXi, VMXm and I23 VMXi, VMXm and I23 teams	
	14:00		
	14:15		
	14:30		
	14:45	Navigating the Diamond cluster Felicity Bertram	
	15:00		
	15:15		
	15:30	Break	
	15:45	follow up Fed ID problems	
	16:00		
	16:15		
	16:30		
	16:45		
	17:00		

Zoom day 2: before data collection

Tue 21st November	
AM CHAIR: David Waterman	
8:30	
8:45	
9:00	
9:15	
9:30	Informal hello/meet & greet
9:45	Welcome & introduction to CCP4 Eugene Krissinel
10:00	
10:15	Introduction to CCP4 interfaces (Cloud/ccp4i2) - setup accounts and run tutorial data Eugene Krissinel / Maria Fando
10:30	
10:45	
11:00	
11:15	Break
11:30	Introduction to space groups Andrey Lebedev
11:45	
12:00	
12:15	
12:30	Lunch
12:45	
13:00	
PM CHAIR: Marco Mazzorana	
13:15	Data Collection Strategies for Photon Counting Detectors Graeme Winter
13:30	
13:45	
14:00	Radiation damage Elspeth Garman
14:15	
14:30	
14:45	Dose driven data collection to optimise your experiments David Aragão
15:00	
15:15	
15:30	Break
15:45	Data Processing (inc scaling) Ana Gonzalez
16:00	
16:15	
16:30	
16:45	
17:00	

Diamond-CCP4 Data Collection & Structure Solution Workshop 2023

Week 1: data collection and processing, phasing

Data collection

Data processing

Experimental phasing

Molecular replacement

MR / model building

Talks		Sun 26th November	Mon 27th November	Tue 28th November	Wed 29th November	Thu 30th November	Fri 1st December				
Practical	ARRIVAL	AM CHAIR: James Beilsten-Edmands		AM CHAIR: Pierre Aller		AM CHAIR: Alex Dias		AM CHAIR: James Parkhurst		AM CHAIR: Adam Crawshaw	
Break		8:30		8:30		8:30		8:30		8:30	
Social		8:45		8:45		8:45		8:45		8:45	
		X35 08:47 bus		X35 08:47 bus		X35 08:47 bus		X35 08:47 bus		X35 08:47 bus	
		9:00		9:00		9:00		9:00		9:00	
		9:15		9:15		9:15		9:15		9:15	
		9:30		9:30		9:30		9:30		9:30	
		9:45		9:45		9:45		9:45		9:45	
		10:00		10:00		10:00		10:00		10:00	
		10:15		10:15		10:15		10:15		10:15	
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		12:15		12:15		12:15		12:15		12:15	
		12:30		12:30		12:30		12:30		12:30	
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				PM CHAIR: Anastasya Shilova		PM CHAIR: David Waterman		PM CHAIR: Maria Fando		PM CHAIR: Blake Balcomb	
		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	
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		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		15:00	
15:15		15:15		15:15		15:15		15:15		15:15	
15:30		15:30		15:30		15:30		15:30		15:30	
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20:00	20:00		20:00		20:00		20:00		20:00		
20:15	20:15		20:15		20:15		20:15		20:15		
		Coach to The Bear		X35 20:16 bus		X35 20:16 bus		X35 20:16 bus			

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Week 2: model building, refinement and validation

Model building / refinement

Model building / validation

Wrap up

Talks	Sat 2nd December	Sun 3rd December	Mon 4th December	Tue 5th December
Practical	Free day	AM CHAIR: Ramona Duman	AM CHAIR: Ramona Duman	AM CHAIR: Anna Warren
Break		8:30	8:30	8:30
Social		8:45	8:45	8:45
		9:00	X35 08:47 bus	X35 08:47 bus
		9:00		9:00
		9:15		9:15
		9:30	Coach from The Bear	
		9:30	Model validation, optimisation and deposition	MX from an Industrial Perspective
		9:45		9:45
		10:00	Robbie Joosten	Ailsa Powell
		10:00		10:00
		10:15	New developments in model building and validation	Analysis tools in CCP4 (PISA, Gesamt, cloud...) and deposition
		10:30		10:15
		10:45	Grzegorz Chojnowski	10:30
		11:00	Break	10:45
		11:00		11:00
		11:15	Crystallography of nucleic acids (tools and practical)	Break
		11:15		11:15
		11:30	Megan Lambert	Future of structural biology
		11:30		11:30
		11:45	Announce Poster Session Winner	11:45
		12:00	Beamline specific talk	12:00
		12:00		HeXI - Alistair Siebert
		12:15	Beamline specific talk	12:15
		12:30	Lunch	Lunch
		12:45		12:30
		13:00		12:45
				13:00
		PM CHAIR: Kamel El Omari	PM CHAIR: Mike Hough	
		13:15		13:15
		13:30	CCP4MG practical	13:30
		13:30		13:45
		13:45	Stuart McNicholas	14:00
		14:00		14:15
		14:15	Work on your own data	14:30
		14:30		14:45
		14:45		15:00
		15:00		15:15
		15:15		15:30
		15:30	Break	15:45
		15:45		16:00
		16:00	Break	16:15
		16:15		16:30
		16:30		16:45
		16:45		17:00
		17:00	Work on your own data	17:15
		17:15		17:30
		17:30		17:45
		17:45		18:00
		18:00		18:15
		EVE CHAIR:	X35 18:25 bus	18:30
		18:15		18:45
		18:30	X35 18:55 bus	19:00
		18:45		19:15
		19:00		19:30
		19:15	Workshop Dinner	19:45
		19:30	Wildwood Kitchen	20:00
		19:45		20:15
		20:00		
		20:15	Coach to The Bear	