

Diamond-CCP4 Data Collection & Structure Solution Workshop 2024

Zoom day 1: before fishing crystals

Talks	Tues 29th Oct	
Practical	AM CHAIR:	
Break	8:30	
Social	8:45	
	9:00	
	9:15	
	9:30	Informal hello/meet & greet
	9:45	Roadmap for the workshop
	10:00	David & Maria
	10:15	MX at Diamond and INSTRUCT-ERIC
	10:30	Marco Mazzorana
	10:45	
	11:00	Break
	11:15	Navigating Diamond SynchWeb and test log
	11:30	in - Marco
	11:45	Navigating the Diamond cluster
	12:00	Felicity Bertram
	12:15	
	12:30	Lunch
	12:45	
	13:00	
	PM CHAIR:	
	13:15	Optimising the Diamond experience
	13:30	David Lawson
	13:45	
	14:00	Cryocrystallography
	14:15	Elspeth Garman
	14:30	
	14:45	Break
	15:00	follow up Fed ID problems
	15:15	
	15:30	
	15:45	
	16:00	
	16:15	
	16:30	
	16:45	
	17:00	

Zoom day 2: before data collection

Tues 19th Nov	
AM CHAIR: Chris	
8:30	
8:45	
9:00	
9:15	Informal housekeeping
9:30	Welcome & introduction to CCP4
9:45	Eugene Krissinel
10:00	Intro to Cloud and homework
10:15	Maria Fando
10:30	Break
10:45	
11:00	Basic Diffraction Theory
11:15	Kamel El Omari
11:30	
11:45	Data Collection Strategies for Photon
12:00	Counting Detectors
12:15	Sofia Trampari
12:30	
12:45	Lunch
13:00	
PM CHAIR: Chris	
13:15	
13:30	Data Processing (inc scaling)
13:45	Ana Gonzalez
14:00	
14:15	Break
14:30	Radiation damage
14:45	Elspeth Garman
15:00	
15:15	Dose driven data collection to optimise
15:30	your experiments
15:45	David Aragão
16:00	
16:15	
16:30	
16:45	
17:00	

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Week 1: data collection and processing, phasing

Week 1: data collection and processing, phasing		Data collection		Data processing		Phasing		Molecular replacement		MR / model building			
Talks	Sun 24th Nov	Mon 25th Nov		Tue 26th Nov		Wed 27th Nov		Thu 28th Nov		Fri 29th Nov			
Practical	ARRIVAL	AM CHAIR: Chris Orr		AM CHAIR: Anna Warren		AM CHAIR: Maria Fando		AM CHAIR: Charles Ballard		AM CHAIR: Charles Ballard			
Break		8:30		8:30		8:30		8:30		8:30			
Social		8:45	X35 08:32 bus	8:45	X35 08:32 bus	8:45	X35 08:32 bus	8:45	X35 08:32 bus	8:45	X35 08:32 bus		
		9:00		9:00		9:00		9:00		9:00			
		9:15	XDS (demo/tutorial) Kay Diederichs	9:15	Intro to space groups and symmetry Andrey Lebedev	9:15	Pathologies and pseudosymmetry Andrey Lebedev	9:15	MX from an Industrial Perspective Judit	9:15	Model building and DM Paul Bond		
		9:30		9:30		9:30		9:30		9:30			
		9:45		9:45		9:45		9:45		9:45			
		10:00	Data Collection and Processing	10:00	Assessing data quality Kay Diederichs	10:00	The phase problem Ed Lowe	10:00	An intro to Moorhen - Lucrezia	10:00	New developments in model building and validation Grzegorz Chojnowski		
		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	DIALS (demo/tutorial) DIALS team	11:00	Break	11:00	Break	11:00	Break	11:00	Break		
		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	I24 - Danny Axford	12:00	VMXi - Halina Mikolajek	12:00	MPL - Andrew Quigley	12:00	VMXm - Anna Warren		
		12:15	Lunch	12:15	Lunch	12:15	Lunch	12:15	Lunch	12:15	Lunch		
		12:30		12:30		12:30		12:30		12:30			
		12:45		12:45		12:45		12:45		12:45			
				PM CHAIR: David Waterman		PM CHAIR: Chris Orr		PM CHAIR: Jose Brandao		PM CHAIR: Jose Brandao			
		13:00	Data Collection and Processing	13:00	Your data in CCP4 Cloud Jools Wills	13:00	Anomalous diffraction in 2024 Ramona Duman	13:00	AlphaFold use for experimental structural biology Oleg Kovalevskiy (Zoom)	13:00	XChem - Daren & Blake		
		13:15		13:15	13:15	13:15	13:15	13:15	13:15	13:15			
		13:30		13:30	Data processing / work on your own data	13:30	An introduction to Coot Judit Debreczeni	13:30	Bioinformatics for structural biologists Dan Rigden (Zoom)	13:30	Ligand Tutorial Daren Fearon / Blake Balcomb		
		13:45		13:45		13:45		13:45		13:45		13:45	
		14:00		14:00		14:00		14:00		14:00		14:00	
		14:15		14:15		14:15		14:15		14:15		14:15	
		14:30		14:30	Coot demo/tutorial Judit Debreczeni	14:30	Coot demo/tutorial Judit Debreczeni	14:30	MR with AlphaFold in CCP4 Cloud (demo/tutorial) Ronan Keegan	14:30	Verification Iracema Caballero		
		14:45		14:45		14:45		14:45		14:45		14:45	
		15:00		Data Collection and Processing	15:00	Break	15:00	Break	15:00	Break	15:00	Break	
		15:15			15:15		15:15		15:15		15:15		15:15
		15:30	15:30		Work on your own data	15:30	Molecular replacement Airlie McCoy	15:30	MR in CCP4 (demo/tutorial) Michail Isupov	15:30	Work on your own data		
		15:45	15:45			15:45		15:45		15:45		15:45	
		16:00	16:00			16:00		16:00		16:00		16:00	
		16:15	16:15			16:15		16:15		16:15		16:15	
		16:30	16:30		Twinning Andrea Thorn (Zoom)	16:30	Work on your own data	16:30	Work on your own data	16:30			
		16:45	16:45			16:45		16:45		16:45			
		17:00	17:00		Poster session with drinks Diamond Atrium	17:00		Work on your own data		17:00		Work on your own data	17:00
		17:15	17:15			17:15				17:15			17:15
		17:30	17:30	17:30		17:30				17:30			
		17:45	17:45	17:45		17:45				17:45			
		18:00	Dinner	18:00	Dinner	18:00	Dinner	18:00	Dinner	18:00			
		18:15		18:15		18:15		18:15		18:15			
		18:30		18:30		18:30		18:30		18:30			
		18:45		18:45		18:45		18:45		18:45			
		19:00		19:00	Poster session with drinks Diamond Atrium	19:00	Work on your own data	19:00	Work on your own data	19:00			
		19:15		19:15		19:15		19:15		19:15			
		19:30		19:30		19:30		19:30		19:30			
		19:45		19:45		19:45		19:45		19:45			
		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	20:15	X35 20:18 bus	20:15	X35 20:18 bus	20:15	X35 20:18 bus	20:15	X35 20:18 bus		

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Week 2: model building, refinement and validation Refinement Model building / validation Wrap up

Talks	Sat 30th Nov	Sun 1st Dec	Mon 2nd Dec	Tue 3rd Dec
Practical	Free day	AM CHAIR: Paul Bond	AM CHAIR: Pierre Aller	
Break		8:30	8:30	8:30
Social		8:45	8:45	8:45
		9:00	X35 08:32 bus	9:00
		9:15		9:15
		9:30	Model validation, optimisation and deposition	9:30
		9:45	Robbie Joosten	9:45
		10:00		10:00
		10:15	Carbohydrate crystallography (tools and practical)	10:15
		10:30	Lucy Schofield	10:30
		10:45		10:45
		11:00	Break	11:00
		11:15	Carbohydrate crystallography (practical)	11:15
		11:30	Jordan Dialpuri	11:30
		11:45		11:45
		12:00	Announce Poster Session Winner	12:00
		12:15	HeXI - Alistair Siebert	12:15
		12:30		12:30
		12:45	Lunch	12:45
		13:00		13:00
		PM CHAIR: Dave Hall	PM CHAIR: Hans Pfalzgraf	
		13:15	13:15	
		13:30	Analysis tools in CCP4 (PISA, Gesamt, cloud...) and deposition	
		13:45	Eugene Krissinel (Zoom)	
		14:00		
		14:15	Refinement case studies	
		14:30	Clemens Vonnrhein (Zoom)	
		14:45		
		15:00	Break	
		15:15		
		15:30	Tutorial - BUSTER	
		15:45	Clemens Vonnrhein (Zoom)	
		16:00		
		16:15		
		16:30		
		16:45		
		17:00	Work on your own data	
		17:15		
		17:30		
		17:45		
		18:00		
		EVE CHAIR:	18:15	X35 18:25 bus
		18:15	18:30	
		18:30		X35 18:54 bus
		18:45		
		19:00		
		19:15		
		19:30	Workshop Dinner	
		19:45	Wildwood Kitchen	
		20:00		
		20:15		
		Coach to The Bear		