

# Diamond-CCP4 Data Collection & Structure Solution Workshop

Online programme, Setup day: Tuesday 23 November

Tuesday 23 November			
AM CHAIR: Elliot Nelson			
8:30		<div>Talks</div> <div>Practical</div> <div>Break</div> <div>Social</div>	
8:45			
9:00			
9:15			
9:30			
9:45			
10:00			
10:15			
10:30			Informal hello/meet & greet
10:45			Welcome - D. Waterman
11:00	Navigating the Diamond cluster F. Bertram		
11:15			
11:30			
11:45	Breakout sessions to confirm sw installation, NX connection and data uploads.		
12:00			
12:15	Lunch		
12:30			
12:45			
PM CHAIR: Ronan Keegan			
13:00	Linux command line scripting G. Winter		
13:15			
13:30			
13:45	Intro to CCP4 Cloud Eugene Krissinel, Andrey Lebedev		
14:00			
14:15			
14:30	Navigating Diamond SynchWeb M. Mazzorana		
14:45			
15:00	Solve outstanding participant problems		
15:15			
15:30			
15:45			
16:00			
16:15			
16:30			
16:45			
17:00			

# Diamond-CCP4 Data Collection & Structure Solution Workshop

Online programme, 1st week: Monday 29 November - Friday 3 December 2021

Monday 29 November		Tuesday 30 November		Wednesday 1 December		Thursday 2 December			Friday 3 December				
AM CHAIR: Felicity Bertram		AM CHAIR: Martin Walsh		AM CHAIR: Marco Mazzorana		BEAMLINE DAY			AM CHAIR: Allen M Orville / Felicity Bertram				
8:30	Informal hello/meet & greet	8:30		8:30		8:30			8:30				
8:45		8:45	Informal Q&A	8:45	Informal Q&A	8:45			8:45	Informal Q&A			
9:00	Introduction to CCP4, CCP4 Cloud Eugene Krissinel	9:00				9:00	Informal Q&A	9:00	More on symmetry and space groups Andrea Thorn		work on your data	9:00	Informal Q&A
9:15		9:15	Data Processing with DIALS Graeme Winter	9:15	Introduction to space groups Andrey Lebedev	9:15		9:15		9:15		The phase problem Ed Lowe	
9:30		9:30		9:30		9:30		9:30		9:30			
9:45	MX at Diamond	9:45		9:45		9:45			9:45				
10:00	Marco Mazzorana	10:00		10:00		10:00			Data Collection		10:00		
10:15	Optimising the Diamond experience David Lawson	10:15	Data Processing with XDS Kay Diederichs	10:15	Break	10:15	10:15	10:15			SHELX for EP Isabel Usón		
10:30		10:30		10:30		10:30	10:30	10:30					
10:45	Break	10:45				10:45	Twinning Andrea Thorn	10:45			10:45	Break	
11:00	Basic Diffraction Theory Kamel El Omari	11:00			11:00			11:00			11:00	11:00	
11:15		11:15	Data Reduction James Beilsten-Edmands	11:15	MX from an Industrial Perspective Ailsa Powell	11:15	Lunch	11:15			Experimental phasing case studies Erika Mancini		
11:30		11:30		11:30		11:30		11:30	11:30	11:30			
11:45		11:45		11:45		Break		11:45	11:45	11:45		11:45	
12:00	Lunch	12:00	Assessing data quality Kay Diederichs	12:00	An introduction to Coot Judit Debreczeni	12:00		Lunch	12:00	SHARP Clemens Vornrhein			
12:15		12:15		12:15		12:15	12:15		12:15		12:15		
12:30		12:30		12:30		12:30	12:30		12:30		12:30		
12:45		12:45	Lunch	12:45	Lunch	12:45	Data Collection		12:45	Lunch			
PM CHAIR: Halina Mikolajek		13:00		13:00		13:00		13:00	13:00		13:00		
13:00	Getting the best from photon counting detectors	13:15		Lunch		13:15		Lunch	13:15		13:15	13:15	
13:15		13:30	13:30		13:30	13:30			13:30		13:30		
13:30	Graeme Winter	PM CHAIR: Anat Shahrar		PM CHAIR: Elliot Nelson		13:45	Data Collection		PM CHAIR: James Beilsten-Edmands				
13:45	Data Collection Strategies David Aragão	13:45	Multi-crystal approaches Selina Storm & DIALS team	13:45	Pathologies and pseudosymmetry Andrey Lebedev	14:00			13:45	Crank 2 Navraj S. Pannu			
14:00		14:00		14:00		14:15			14:00		14:15		
14:15		14:15		14:15		14:15			14:30		14:15		
14:30	Break	14:30		14:30	Remarks and discussions about resolution, data quality and all that Clemens Vornrhein	14:45	14:30	EP Tutorials					
14:45	Cryocrystallography Elspeth Garman	14:45	Break	14:45	Break	15:00	14:45						
15:00		15:00	Data processing tutorials (data reduction / quality stats /multiple datasets)	15:00		Break	15:15		15:00				
15:15		15:15		15:15	15:15		15:15	15:15					
15:30	Break	15:30		Practical/own data time?	15:30	15:45	15:30	Break					
15:45	Radiation damage Elspeth Garman	15:45			15:45	16:00	15:45	15:45	Work on your own data				
16:00		16:00			16:00	16:15	16:00	16:00					
16:15		16:15			16:15	16:30	16:15	16:15					
16:30	VMXm	16:30			16:30	16:45	16:30	Work on your own data					
16:45	Anna Warren	16:45			16:45	17:00	16:45						
17:00		17:00		17:00			17:00						

# Diamond-CCP4 Data Collection & Structure Solution Workshop

Online programme, 2nd week: Monday 6 - Friday 10 December 2021

Monday 6 December			Tuesday 7 December			Wednesday 8 December			Thursday 9 December			Friday 10 December			
AM CHAIR: Ramona Duman			AM CHAIR: Dave Hall			AM CHAIR: Sam Horrell			AM CHAIR: Armin Wagner			AM CHAIR: Danny Axford			
8:30			8:30			8:30			8:30			8:30			
8:45	Welcome back to Week 2		8:45	Informal Q&A		8:45	Informal Q&A		8:45	Informal Q&A		8:45	Informal Q&A		
9:00			9:00			9:00			9:00			9:00			
9:15	MR introduction and theory Michail Isupov		9:15	I23		9:15			9:15			9:15			
9:30			9:30	Ramona Duman		9:30	DM		9:30	Model validation and optimisation		9:30	CCP4MG		
9:45			9:45			9:45	Kevin Cowtan		9:45	Robbie Joosten		9:45	Stuart McNicholas		
10:00	Molecular replacement case studies		10:00	XFEL Hub Jos Kamps		10:00	Model building (buccaneer and modelcraft)		10:00	VMXi / Crystallisation facility		10:00	cryoEM		
10:15	Paula Salgado		10:15	Break		10:15			10:15	Juan Sanchez-Weatherby &		10:15	Ana Casañal		
10:30	Break		10:30	MR model selection, preparation and assessing the solution		10:30	Paul Bond		10:30	Halina Mikolajek		10:30	Break		
10:45	Work on your own data		10:45				10:45	Break		10:45	Break		10:45	microED	
11:00			11:00		Ronan Keegan		11:00			11:00		Adam Crawshaw			
11:15				11:15	Break		11:15	Model Building (arpwarp / shelxe)		11:15	Aleph		11:15	Machine Learning	
11:30			11:30			11:30	(arpwarp / shelxe)		11:30	Massimo Sammito		11:30	Melanie Vollmar		
11:45	Break		11:45	Advanced molecular replacement		11:45	Isabel Usón		11:45	Announce Poster Session Winner		11:45	CCP4MG practical		
12:00	MR with Phaser: Part 1 Airlie McCoy		12:00	Claudia Millán		12:00	REFMAC Lucrezia Catapano		12:00	Tutorial - BUSTER		12:00	Stuart McNicholas		
12:15			12:15	Lunch		12:15			12:15	Clemens Vornrhein		12:15	Lunch		
12:30			12:30			12:30			12:30		12:30				
12:45	Lunch		12:45			12:45		12:45		12:45		12:45			
13:00			13:00		13:00		13:00		13:00		13:00				
13:15			PM CHAIR: Mike Hough			13:15	Lunch		13:15		PM CHAIRS: M. Mazzorana, R. Duman, D. Waterman, J. Parkhurst & M. Vollmar				
13:30		13:15		13:30		PM CHAIR: Adam Crawshaw			13:15						
PM CHAIR: Kyle Stevenson			13:30	Advanced Coot and ligand fitting Daren Fearon		PM CHAIR: Halina Mikolajek			13:30	PISA Eugene Krissinel		13:30	Work on your own data		
13:45	MR with Phaser: Part 2 Airlie McCoy		13:45			13:45		13:45			13:45				
14:00			14:00	Ligand Tutorial Daren Fearon	14:00	BUSTER Clemens Vornrhein	14:00		14:00						
14:15			14:15				14:15		14:15	Work on your own data	14:15				
14:30	Break		14:30	Charlie Tomlinson		14:30	REFMAC tutorial Robert Nicholls		14:30	Work on your own data		14:30	Student feedback session - 5 min presentations		
14:45	MR Tutorials		14:45	Break	14:45			14:45			14:45				
15:00			15:00			15:00			15:00			15:00			
15:15			15:15	Bioinformatics for structural biologists	15:15	Break	15:15	Break	15:15	Break	15:15	Wrap up from organisers			
15:30		15:30			15:30				15:30	AlphaFold DB	15:30	Break			
15:45	Break	15:45	Daniel Rigden		15:45		Work on your own data		15:45	Sameer Velankar	15:45	Work on your own data	15:45		
16:00	Work on your own data	16:00	Model prediction using colab servers Claudia Millán Paula Salgado	16:00		16:00		Work on your own data	16:00		16:00				
16:15				16:15		16:15				16:15					
16:30				16:30		16:30				16:30					
16:45			16:45	Work on your own data	16:45				16:45		16:45				
17:00			17:00			17:00				17:00			17:00		

Talks
Practical
Break
Social