

Diamond-CCP4 Data Collection & Structure Solution Workshop
 Online programme, 1st week: Monday 30 November - Friday 4 December 2020

Monday 23 November - Set up 'drop in session' for attendees, timings tbc

Monday 30 November		Tuesday 1 December		Wednesday 2 December		Thursday 3 December		Friday 4 December	
AM CHAIR:		AM CHAIR:				AM CHAIR:		AM CHAIR:	
08:30	Informal hello/meet & greet	08:30		08:30		08:30		08:30	
08:45		08:45	Informal Q&A	08:45	Informal Q&A	08:45		08:45	Informal Q&A
09:00	Welcome (30 mins) Eugene Krissinel	09:00	Data Collection Strategies (45 mins) David Arago	09:00	Introduction to space groups (1hr) Andrey Lebedev	Data Collection		09:00	The phase problem (45 mins) Ed Lowe
09:15	09:15	09:15		09:15					
09:30	MX at Diamond (30 mins) Marco Mazzorana	09:30	09:30	09:30					
09:45	09:45	09:45	09:45						
10:00	Optimising the Diamond experience (30 mins) David Lawson	10:00	10:00	10:00					
10:15	10:15	10:15	10:15	10:15					
10:30	Break (30 mins)	10:30	10:30	10:30					
10:45	10:45	10:45	10:45	10:45					
11:00	Intro to CCP4 Cloud (1hr) Eugene Krissinel, Andrey Lebedev	11:00	11:00	11:00					
11:15		11:15	11:15	11:15					
11:30		11:30	11:30	11:30					
11:45		11:45	11:45	11:45					
12:00	Lunch (1hr)	12:00	12:00	12:00	Lunch (1hr)		12:00	Experimental phasing case studies (45 mins) Paula Salgado	
12:15		12:15	12:15	12:15					
12:30		12:30	12:30	12:30					
12:45		12:45	12:45	12:45					
PM CHAIR:		13:00	Lunch (1hr)	13:00	Lunch (1hr)	Data Collection		13:00	Lunch (1hr)
13:00	Basic Diffraction Theory (1hr) Kamel El Omari	13:15		13:15				13:15	
13:15		13:30		13:30				13:30	
13:30		PM CHAIR:		13:45				PM CHAIR:	
13:45	13:45	13:45	13:45	14:00	14:00	14:00	14:00	14:00	
14:00	Break (15 mins)	14:00	14:00	14:00	14:15	14:15	14:15	14:15	
14:15	Getting the best from photon counting detectors (45 mins) Andreas Förster	14:15	14:15	14:15	14:30	14:30	14:30	14:30	
14:30		14:30	14:30	14:30	14:45	14:45	14:45	14:45	
14:45	14:45	14:45	14:45	14:45	15:00	15:00	15:00	15:00	
15:00	Cryocrystallography (45 mins) Elspeth Garman	15:00	15:00	15:00	15:15	15:15	15:15	15:15	
15:15		15:15	15:15	15:15	15:30	15:30	15:30	15:30	
15:30	15:30	15:30	15:30	15:30	15:45	15:45	15:45	15:45	
15:45	Break (15 mins)	15:45	Data processing tutorials (data reduction / quality stats /multiple datasets) (45 mins) Upload data & Linux tutorial (45 mins)	15:45	Break (30 mins)	Data Collection		15:45	Break (30 mins)
16:00	16:00	16:00		16:00					
16:15	16:15	16:15		16:15					
16:30	16:30	16:30		16:30					
16:45	VMXm (30 mins) Anna Warren	16:45	16:45	16:45	17:00	17:00	17:00	17:00	
17:00		17:00	17:00	17:00	17:00	17:00	17:00	17:00	

Talks
Practical
Break
Social

Diamond-CCP4 Data Collection & Structure Solution Workshop

Online programme, 2nd week: Monday 7 - Friday 11 December 2020

Monday 7 December		Tuesday 8 December		Wednesday 9 December		Thursday 10 December		Friday 11 December	
AM CHAIR:		AM CHAIR:		AM CHAIR:		AM CHAIR:		AM CHAIR:	
08:30		08:30		08:30		08:30		08:30	
08:45	Welcome back to Week 2	08:45	Informal Q&A	08:45	Informal Q&A	08:45	Informal Q&A	08:45	Informal Q&A
09:00		09:00		09:00		09:00		09:00	
09:15	MR introduction and theory (45 mins) Michail Isupov	09:15	I23 (30 mins) Ramona Duman	09:15	DM (45 mins) Kevin Cowtan	09:15	Model validation and optimisation (45 mins) Robbie Joosten	09:15	CCP4MG (45 mins) Stuart McNicholas
09:30		09:30		09:30		09:30			
09:45		09:45	XFEL Hub (30 mins) Agata Butryn	09:45	Automated Model Building (buccaneer / arpwrap / shelxe) (45 mins) Isabel Uson	09:45	VMXi / Crystallisation facility (45 mins) Juan Sanchez-Weatherby & Halina Mikolajek	09:45	cryoEM (30 mins) Ana Casañal
10:00	Molecular replacement case studies (30 mins) Adam Crawshaw	10:00	Break (15 mins)	10:00	Break (30 mins)	10:00	Break (30 mins)	10:00	Machine Learning (30 mins) Melanie Vollmar
10:15		10:15		10:15		10:15			
10:30	Break (15 mins)	10:30	MR model selection, preparation and assessing the solution (45 mins) Ronan Keegan	10:30	REFMAC (45 mins) Robert Nicholls	10:30	Work on your own data (1hr30)	10:30	Work on your own data (1hr)
10:45	Work on your own data (1hr)	10:45	Break (15 mins)	10:45	BUSTER (45 mins) Clemens Vornrhein	10:45		Lunch (1hr)	
11:00		11:00		11:00		11:00			
11:15		11:15	11:15	11:15	11:15				
11:30		11:30	Advanced molecular replacement (45 mins) Michail Isupov	11:30	Lunch (1hr)	11:30	Lunch (1hr)	11:30	Lunch (1hr)
11:45	Break (15 mins)	11:45	Lunch (1hr)	11:45		11:45		11:45	
12:00	Combined Likelihood MR/SAD in Phaser: Part 1 (45 mins) Airlie McCoy	12:00		Lunch (1hr)	12:00	Lunch (1hr)	12:00	Lunch (1hr)	12:00
12:15		12:15	12:15		12:15				
12:30		12:30	Lunch (1hr)	12:30	Lunch (1hr)	12:30	Lunch (1hr)	12:30	Lunch (1hr)
12:45	Lunch (1hr)	12:45		12:45		12:45		12:45	
13:00			13:00	PM CHAIR:	13:00	PM CHAIR:	13:00	PM CHAIR:	13:00
13:15	13:15	13:15	13:15						
13:30		13:30	Advanced Coot and ligand fitting (45 mins) Daren Fearon	13:30	Refinement Tutorials (1hr45)	13:30	PISA (45 mins) Eugene Krissinel	13:30	Work on your own data (1hr)
13:45	Combined Likelihood MR/SAD in Phaser: Part 1 (45 mins) Airlie McCoy	13:45	Ligand Tutorial (45 mins)	13:45		13:45		13:45	
14:00		14:00		14:00	14:00	14:00			
14:15		14:15	Break (30 mins)	14:15	Work on your own data (1hr15)	14:15	Work on your own data (1hr15)	14:15	Student feedback session - 5 min presentations
14:30	Break (15 mins)	14:30		14:30		14:30			
14:45	MR Tutorials (1hr)	14:45	Break (30 mins)	14:45	Break (30 mins)	14:45	Break (30 mins)	14:45	Break (15 mins)
15:00		15:00		15:00		15:00			
15:15		15:15	Work on your own data (2hrs)	15:15	Work on your own data (1hr15)	15:15	Work on your own data (1hr15)	15:15	Student feedback session - 5 min presentations
15:30	Break (15 mins)	15:30		15:30		15:30			
15:45		15:45	Work on your own data (1hr15)	15:45	Work on your own data (1hr15)	15:45	Work on your own data (1hr15)	15:45	Wrap up from organisers
16:00	Work on your own data (1hr15)	16:00		16:00		16:00			
16:15		16:15	Work on your own data (1hr15)	16:15	Work on your own data (1hr15)	16:15	Work on your own data (1hr15)	16:15	Wrap up from organisers
16:30		16:30		16:30		16:30			
16:45		16:45	16:45	16:45	16:45	16:45	16:45	16:45	16:45
17:00		17:00	17:00	17:00	17:00	17:00	17:00	17:00	17:00

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