

Crystallographic Computing School - Bangalore, India (15th-20th August 2017)

Program

Day 1 - August 15th: Basic crystallography and algorithms	Speakers	Time
Introduction		10.15am-10.30am
Macromolecular crystallography: from isolated programs to full package	Eleanor Dodson	10.30am-11.30am
Crystallographic methods: historical perspective	M. R. N. Murthy	11.30am-12.30am
Lunch and Poster session		12.30pm-2pm
Statistics and Bayesian statistics in crystallography	Tom Terwilliger	2pm-3pm
Coffee break		3pm-3.30pm
Structure factor statistics and electron density	Garib Murshudov	3.30pm-4.30pm
Quality of diffraction data	Kay Diederichs	4.30-5.30pm
Tutorials		5.30pm-6.30pm
Dinner		7pm onwards
Day 2 - August 16th: Software development and tools		
Processing data collected with Pilatus/Eiger detectors	James Parkhurst	9.30am-10.30am
Coffee break		10.30am-10.45am
Design of pipelines: Reuse of existing tools	Santosh Panjekar	10.45am-11.45am
High-performance computing using python and OpenCL/ modular approach to crystallographic software development	Vincent Favre- Nicolin	11.45am-12.45pm
Lunch and Poster session		12.45pm-1.45pm
Group photo		1.45pm-2pm
Tutorials		2pm-3pm
Coffee break		3pm-3.15pm
Recent advances in refinement of small molecule structures	Richard Cooper	3.15pm-4.15pm
Singular-value decomposition of Rietveld least-squares matrix	Patrick Mercier	4.15pm-5.15pm
Structure solution from powder data-part I: direct methods	Corrado Cuocci	5.15pm-6.15pm
Dinner		7pm onwards
Day 3 - August 17th: Powder diffraction and structure solution methods		
Algorithms and coding of PDF approach to analyze nanophase materials	Simon Billinge	9.30am-10.30am
Coffee break		10.30am-10.45am
Fundamental parameters approach in X-ray powder diffraction	Marcus Mendenhall	10.45am-11.45am
Structure solution from powder data-part II: real space methods	Corrado Cuocci	11.45am-12.45pm
Lunch and Poster session		12.45pm-2pm
Tutorials	Corrado Cuocci	2pm-3pm
GUI Design: science or psychology	Harry Powell	3:00pm - 4:00pm
IISc Alumni Association Lecture	Eleanor Dodson	4:00pm-5.30pm
Discussions - Software tools and languages in crystallography		6pm-7pm
Dinner		7pm onwards
Day 4 - August 18th		
No Scheduled Lectures		

Day 5 - August 19th: Challenges in crystallographic software development and beyond		
Electron Diffraction data - new perspectives	Lukáš Palatinus	9.30am-10.30am
Coffee break		10.30am-10.45am
Free electron laser data - problems and challenges	Thomas White	10.45am-11.45am
TLS and normal modes	Shekhar Mande	11.45am-12.45pm
Lunch		12.45pm-2pm
Poster Speaker1		2pm-2.20pm
Poster Speaker2		2.20pm-2.40pm
Poster Speaker3		2.40pm-3pm
Neutron diffraction scattering analysis	Simon Billinge	3pm-4pm
Cricket Match IISc Gymkhana grounds 4:30-6:30pm		
Discussions - Challenges in crystallographic computing		7pm-8pm
Dinner		8pm onwards
Day 6 - August 20th		
Breakfast and departure		