Computing in Crystallography Forum Program

Fri 22

19:00	Welcome Cocktail	
20:00	Welcome talk	
20:10	Software development in CCP4	Eugene Krissinel
21:00	Social	

Sat 23

9:30	FlexCryst: An Integrated Software Suite for Crystallographic Analysis – Architecture, Capabilities, and Technical Challenges	Detlef Hofmann
10:00	Beyond IAM: applications of MATTS data bank	Marta Kulik
10:30	Coffee	
11:00	Inferring contact area heterogeneity from static protein conformations	Kliment Olechnovič
11:30	Computing for Coot model building and refinement without the graphical user interface	Lucrezia Catapano
12:00	Ada for teaching, learning and doing crystallography	Saulius Gražulis
12:30	Lunch	
13:30	Problems description	
14:00	Programming session	
16:00	Tea	
16:30	Free discussions/Programming session	
17:40	Scripting through the reciprocal space: on the back alleys of crystallography	Daniel Tchoń

18:00	Fast & Furious Factors: Exploiting Symmetry to Satisfy DiSCaMB's Need for Speed	Lukasz Golon
18:30	Using neural networks to interpret electron density maps for automated atomic model building	Paul Bond
19:00	Dinner	
20:00	Crystallographic Insights into the Digital Reconstruction of Moroccan Geometric Art	El Houcini Ettajer
20:30	social	

Sun 24

9:30	Errors	Martin Lutz
10:30	Coffee	
11:00	Integrating Data Sources in CCP4 Cloud for Online Structure Determination	Jools Wills
11:30	Predicting molecular motions	Sergei Grudinin
12:00	Counterpoint – CASP and the Special Role of Crystallographers in Solving the Protein Folding Problem	Krzysztof Fidelis, Maciej Antczak and Andriy Kryshtafovych
12:30	Lunch	
13:30	Problems description	
14:00	Programming session	
16:00	Tea	
16:30	Programming session	
19:00	Farewell Cocktail	