

CCP-EM / CCP-BioSim Workshop

- *Computation for Biomolecular Cryo-Electron Microscopy and Tomography* -

Astbury Centre | University of Leeds | Friday 14th July | Worsley 9.58c

10:00 Coffee & registration

11:00 Sarah Harris & Tom Burnley (University of Leeds & STFC)

Setting the scene, what are the computational challenges for EM/ET? What can we do with simulation, and what else is needed?

11:20 Remy Martin (Berger-Schaffitzel group, University of Bristol)

An integrated approach to the structure and dynamics of the bacterial holo-translocon

12:00 Agnel Joseph (Topf group, Birkbeck College)

Refinement of atomic models in cryo-EM density using Flex-EM and assessment of fits with TEMPy

12:30 CCP flash presentations & lunch

13:30 Elena Orlova (Birkbeck College)

Cryo EM or X-ray? Challenges, Achievements, and Prospects

14:10 Max Bonomi (Vendruscolo group, University of Cambridge)

Simultaneous determination of protein structure and dynamics using cryo-electron microscopy

14:40 Nvidia hardware presentation

15:00 Coffee break & group discussion

15:30 Tristan Croll (University of Cambridge)

Interactive MD for model building and validation

16:00 Christian Blau (Lindahl Group, Stockholm University)

Bayes' model for the ensemble behind cryo-EM densities

16:30 Jose-Maria Carazo (National Center for Biotechnology, Spain)

Validation and quality control all way through from maps to models