

4th Annual CCP-SAS Project Workshop, June 19-21, 2017

Cardiff University, Cardiff, Wales, UK

Program

Monday June 19, 2017

Community Science Meeting - Beverton Lecture Theatre, Main Building, Cardiff University, Park Place

Registration

08:30 - 09:00 Registration (in the Viriamu Jones Gallery)

Welcomes

09:00 - 09:15 Welcomes

Review of CCP-SAS

- 09:15 - 09:30 The CCP-SAS vision four years later
(Paul Butler, University of Tennessee Knoxville)
- 09:30 - 09:45 Applications and achievements of CCP-SAS
(Stephen Perkins, University College London)
- 09:45 - 10:05 GenApp: The CCP-SAS deployment framework
(Emre Brookes, University of Texas Healthcare Science Center San Antonio)
- 10:05 - 10:25 The SASSIE Portfolio
(Jayesh Bhatt, University College London)

10:30 - 11:00 Refreshments & Posters (Viriamu Jones Gallery)

Applications of CCP-SAS in Biology, Biotechnology and Soft Matter

- 11:00 - 11:15 Experiences of modelling long multi-domain complement proteins
(Amy Osborne, University College London)
- 11:15 - 11:30 SASSIE modelling of human IgE and IgG antibodies
(Jayesh Bhatt, University College London)
- 11:30 - 11:45 Antibody characterisation and interactions
(Monica Castellanos, NIST)
- 11:45 - 12:00 Very wide-angle scattering of neutrons to look at the solvent layer of proteins
(Dave Scott, Nottingham University)
- 12:00 - 12:15 HPC and SASSIE modelling of detergent micelles
(Chris Lorenz, King's College London)
- 12:15 - 12:30 Surfactants and molecular dynamics
(Andrew McCluskey, University of Bath)

12:30 - 13:45 Buffet Lunch and Posters (Viriamu Jones Gallery)

CCP-SAS Going Forward: Developments and Opportunities - I

- 13:45 - 14:00 CCP-BioSim - Successes, challenges and applications
(Sarah Harris, Leeds University)
- 14:00 - 14:15 Determining Minimal Ensemble Models of SAXS Experiments
(Jeff Wereszczynski, Illinois Institute of Technology)
- 14:15 - 14:30 Zebbede: Solvated polymer model construction for comparison with SAS data
(David Willock, Cardiff University)
- 14:30 - 14:45 Multiscale simulations of macromolecules
(Paola Carbone, University of Manchester)
- 14:45 - 15:00 Exploring protein association pathways with time-resolved SAS
(Wojciech Potrzebowski, European Spallation Source)
- 15:00 - 15:15 Discussion

15:00 - 15:30 Refreshments & Posters (Viriamu Jones Gallery)

CCP-SAS Going Forward: Developments and Opportunities - II

- 15:45 – 16:00 Structural refinement in molecular simulations of non-crystalline systems
(*Tom Headen, ISIS Pulsed Neutron Source*)
- 16:00 - 16:15 DL_Software Modelling Capabilities in Molecular Simulations
(*Chin Yong, STFC Scientific Computing Department*)
- 16:15 - 16:30 Computer Aided Formulation (CAF): Industrial needs for CCP-SAS
(*Peter Dowding, Infineum*)
- 16:30 - 16:45 The Facility Perspective
(*Tim Snow, Diamond Light Source*)
- 16:45 - 17:00 Discussion

Departure

17:00 Depart

Tuesday June 20 2017

Project Business Meeting - Room 0.77, Main Building, Cardiff University, Park Place

09:00 - 10:30 Legacy & Succession Planning

10:30 - 11:00 Refreshments

11:00 - 12:30 Moving Forward

12:30 - 13:30 Buffet Lunch

13:30 - 15:00 Closing out the Current Grant

15:00 - 15:30 Refreshments

15:30 - 16:00 Project Team Meeting

Departure

16:00 Depart

Wednesday June 21 2017

Tutorial Sessions - Room 0.77, Main Building, Cardiff University, Park Place

Tutorial (prior registration required)

Please also see Venue & other information for further instructions

09:00 - 12:15 SASSIE for beginners
(*Jayesh Bhatt, Amy Osborne, Andrew McCluskey, Steve Perkins*) - Room 1.25

12:15 – 13:30 Lunch (NB: lunch is not provided)

Tutorials (prior registration required)

Please also see Venue & other information for further instructions

14:00 - 17:15 Introduction to GenApp
(*Emre Brookes*) - Room 0.77

14:00 - 17:15 Advanced use of SASSIE
(*Jayesh Bhatt, Amy Osborne, Andrew McCluskey, Steve Perkins*) - Room 1.25