

CoSeC Conference 2023
 Wednesday 6 December
 Manchester Central Convention Complex
AGENDA



TIME	SPEAKER	PRESENTATION TITLE
10:00 - 10:10	Stephen Longshaw (CoSeC Technical Lead, UKRI STFC)	Welcome and Introduction
10:10 - 11:10	Computational Engineering	
10:10 - 10:25	Ajay Harish (The University of Manchester)	Digital Wave Flume Using Multi-Fidelity Approaches
10:25 - 10:40	Mark Pellowe (Loughborough University)	An Adaptive Cost Function for the Multi-Fidelity Optimisation of Engineering Problems
10:40 - 10:55	Omar Ahmed Mahfoze (UKRI STFC)	Multiscale Universal Interface for Heterogeneous High-Performance Computing Systems
10:55 - 11:10	Chaired panel discussion	
11:10 - 11:30	REFRESHMENTS	
11:30 - 12:30	Scientific Reproducibility	
11:30 - 11:45	Jas Kalayan (UKRI STFC)	FAIR Data for the Biomolecular Simulation Community
11:45 - 12:00	Jörg Saßmannshausen (Imperial College London)	Scientific Reproducibility: The importance of reliable and sustainable software installation
12:00 - 12:15	Alin Elena (UKRI STFC)	PSDI: Data to Knowledge
12:15 - 12:30	Chaired panel discussion	
12:30 - 13:30	LUNCH BREAK	
13:30 - 14:45	High Performance & Future Computing	
13:30 - 13:45	Harvey Devereux (Queen Mary University London)	Calculating system properties on-the-fly in DL_POLY
13:45 - 14:00	Maria Panoukidou (University of Edinburgh)	Runaway Transition in Irreversible Polymer Condensation with Cyclisation
14:00 - 14:15	Michael Seaton (UKRI STFC)	Thermodynamically consistent multi-phase DPD
14:15 - 14:30	Marcello Puligheddu (UKRI STFC)	Acceleration of Electronic Structure Codes on Heterogeneous Hardware
14:30 - 14:45	Chaired panel discussion	

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TIME	SPEAKER	PRESENTATION TITLE
14:45 - 15:30	Tomographic Imaging and Reproduction	
14:45 - 15:00	Laura Murgatroyd (UKRI STFC)	Reproducible Tomographic Image processing with CIL
15:00 - 15:15	William Lionheart (The University of Manchester)	Computational Challenges in Rich Tomography — creating an integrated computational framework for simultaneous CT modelling and reconstruction
15:15 - 15:30	Chaired panel discussion	
15:30 - 16:00	REFRESHMENTS	
16:00 - 17:00	CoSeC Past / Present / Future	
16:00 - 16:30	David Emerson (UKRI STFC)	From Concept to CoSeC: A CCP Tale
16:30 - 17:00	Stephen Longshaw (CoSeC Technical Lead, UKRI STFC)	CoSeC: Now and the Future
17:00 - 17:30	Community feedback session and wrap-up (chaired)	