

# CoSeC Conference 2022

Thursday 1 December  
Manchester Central



Annual Conference 2022

Thursday 1 December @ CIUK 2022

## AGENDA

TIME	SPEAKER	PRESENTATION TITLE
09:30 - 09:45	Barbara Montanari (Director CoSeC, STFC)	Welcome and Introduction
<b>09:45 - 11:15</b>	<b>Data Science &amp; Machine Learning</b>	
09:45 - 10:15	Stefano Mensa (Hartree Centre)	Quantum Machine Learning Framework for Virtual Screening in Drug Discovery: a Prospective Quantum Advantage
10:15 - 10:45	Jiayun Pang (University of Greenwich)	A Natural Language Processing (NLP)-Based Deep Learning Approach to Predict Solubility Parameters for Drug Discovery
10:45 - 11:15	Yuhan Wang (University College London)	Using molecular dynamics simulation to predict the aggregation propensity of mAb formulations & accelerate development
11:15 - 11:45	<b>REFRESHMENTS</b>	
<b>11:45 - 13:15</b>	<b>Coupling &amp; Data Workflows</b>	
11:45 - 12:15	Wendi Liu (STFC)	ParaSiF: A Partitioned Fluid-Structure Interaction Simulation Framework
12:15 - 12:45	Raz Benson (University College London)	Fast pattern detection in kinetic Monte Carlo simulations of heterogeneous catalysis
12:45 - 13:15	Chien Nguyen (Bangor University)	Reusing Previous Simulation Runs: Applications in Environmental Fluid Dynamics
13:15 - 14:00	<b>LUNCH BREAK</b>	
<b>14:00 - 16:00</b>	<b>High Performance &amp; Future Computing</b>	
14:00 - 14:30	Stefano Rolfo (STFC)	Modernisation of the 2DECOMP&FFT Library for Hybrid Architecture
14:30 - 15:00	Jianping Meng (STFC)	Domain specific languages for exascale fluid simulations
15:00 - 15:30	Jian Fang (STFC)	Study of High-Speed Aerodynamics based on High-Fidelity Simulation
<b>15:30 - 16:00</b>	<b>Panel Discussion and Wrap Up</b>	
15:30 - 15:55	Panel Discussion (Chair: Sylvain Laizet)	
15:55 - 16:00	Stephen Longshaw (STFC)	Wrap Up