



CoSeC@CIUK – 9th December 2021, Manchester Central

Session 1: Introducing CoSeC

- 10:00 - 10:20: **Introduction to CoSeC** (Barbara Montanari, *CoSeC director*)
- 10:20 - 10:40: **Software citation & cataloguing** (Alejandra Gonzales-Beltran & Gemma Poulter, *Data & Software Engineering Group*)
- 10:40 - 11:00: **CoSeC impact activities and wider lessons learned** (Dawn Geatches, *CoSeC project office*)

11:00 - 11:30 - Break

Session 2: Exascale Computing

- 11:30 - 11:50: **A Million Cores and Beyond: Opportunities and Outlook for Exascale Computing** (David Emerson, *Computational Engineering Group*)
- 11:50 - 12:10: **Materials modelling and particle simulations at exascale** (Phil Hasnip, *University of York*)
- 12:10 - 12:30: **CRYSTAL22 - Thanks for the memory** (Ian Bush, *Theoretical & Computational Physics Group*)

12:30 - 13:30 - Lunch

13:30 - 14:30: Data Science

- 13:30 - 13:50: **CoVal: Understanding SARS-CoV-2 variants by integrating genome and 3D structure data** (Agnel-Praveen Joseph, *Biology and Life Sciences Group*)
- 13:50 - 14:10: **The CCPi core imaging library, a versatile software for tomographic imaging** (Edoardo Pasca, *Biology and Life Sciences Group*)
- 14:10 - 14:30: **Simulation meets Machine Learning for supercharging science** (Keith Butler, *Scientific Machine Learning Group*)

14:30 - 15:00 - Break

Session 3: Scientific Challenges

- 15:00 - 15:20: **Nuclear thermal hydraulics for low-carbon applications - understanding energy and mass transport in advanced nuclear reactor systems** (Wei Wang, *Computational Engineering Group*)
- 15:20 - 15:40: **Towards a quantum annealing algorithm for determining crystal structures** (Ronan Keegan, *Biology and Life Sciences Group & Adam Callison, University College London*)
- 15:40 - 16:00: **Machine Learning for interatomic potentials** (Alin Elena, *Computational Chemistry Group*)

