31st MCC Meeting

12 July 2021

Agenda

10:25 Scientific Programme

10:30 ARCHER2 update (Holly Judge, EPCC)

10:45 Developing systematically improvable and practical post-DFT approaches for materials – new member code boo (George Booth, Department of Physics, King's College London)

11:00 An investigation of NH_3-SCR of NOx mechanism over Cu-CHA by a hybrid QM/MM Embedded Technique – group member code cat (Jamal Abdul Nasir, Department of Chemistry, UCL)

11:15 Gecko's: How do they do that? – group member code shu (Ian Shuttleworth, School of Science and Technology, University of Nottingham Trent)

11:30 Bede, the N8-based tier-2 supercomputer that is based upon Power+GPU architecture - invited speaker from N8 (Matthew Probert, Department of Physics, University of York)

11:40 CASTEP on ARCHER2 - invited speaker from UKCP (Phil Hasnip, Department of Physics, University of York)

12:00 Lunch break

13:30 Main MCC Business Meeting

1   Messages
2   Annual Reports
3   New Members
4   National HPC Resources
5   Excalibur – update from MMM DDWG
6   Proposals Supported
7   MCC usage of Allocated Resources
8   Distribution of Resources: new proposals
9   Any other business

15:00 Close