





## Celebration of Science



## Lightning Talks

	Poster Presenter	Poster Title
1	Ben Durham, University of York	Open Boundary Conditions and Implicit Solvation Calculations in CASTEP using DL MG
2	Callum Watson, British Geological Survey	Enabling a better global view of the magnetic field of Earth's rocks
3	Carlos Edgar Lopez Barrera, Queen Mary University of London	Computational Insights for Individualized Atrial Fibrillation Treatments
4	Chi Cheng (Cecilian) Hong, University of Edinburgh	Insight into the Correlated Disorder of Fumarate- Based MIL- 53 Frameworks: A Computational Study of Free-Energy Landscape
5	Ivan Tolkachev, University of Oxford	Large scale atomistic simulations of nanocrystalline Iron formation and its irradiation performance
6	Joel Hirst, Sheffield Hallam University	Spin-Waves: A potential route to more efficient data transmission, storage and processing
7	Joseph Prentice, University of Oxford	Computing infra-red spectra using finite differencing in CASTEP
8	Juan Herrera, EPCC, The University of Edinburgh	MONC Performance Portability
9	Kevin Stratford, EPCC, The University of Edinburgh	MPI+X on ARCHER2: observations from Ludwig
10	Ludovica Cicci, Imperial College London	A multi-scale analysis of the impact of measurement and physiological uncertainty on electrocardiograms
11	Mara Strungaru, University of York	Implementing spin-lattice dynamics within the VAMPIRE software package
12	Marina Strocchi, Imperial College London & King's College London	Linking Molecular to Whole-organ Function Using Multi-scale, Multi-physics Four-chamber Computational Models
13	Martin Plummer, STFC Scientific Computing Department (Daresbury Laboratory)	Multi-Layered MPI parallelisation for the R-matrix with time- dependence code
14	Matt Smith, University of York	Future-proof Parallelism for Plane-Wave Density Functional Theory
15	Matthias Frey, University of St Andrews	EPIC: The Elliptical Parcel-In-Cell method
16	-	
17	Paul Bartholomew, EPCC, University of Edinburgh	Adding ADIOS2 to the Xcompact3D CFD code
18	Pavel Stishenko, Cardiff University	Implementing an implicit solvent model in a periodic DFT code
19	Sean Mashallsay, Queen's University Belfast	Unravelling Attosecond Dynamics: A General Approach To Ultrafast Atomic Simulations
20	Steven Boeing, University of Leeds	Small-scale mixing in a parcel-based model of moist convection
21	Stuart Morris, University of Warwick	Laser-plasma instabilities at Shock Ignition scales
22	Tobias Slade-Harajda, University of Warwick	The consequences of tritium mix for simulated ion cyclotron emission spectra from deuterium-tritium plasmas
23	Vinush Vigneswaran, The University of Edinburgh – Centre for Cardiovascular Science	OpenEP Workbench: A computational platform for identifying fibrotic regions and conduction disturbances in the atria using conduction velocity.
24	Hannah Menke, Heriot-Watt University	Introducing GeoChemFoam to Archer2
25	Nick Brown, EPCC, The University of Edinburgh	ExCALIBUR: An exascale software programme